

Jan Delaval

Access DB# 75515

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: S. Kumar Examiner #: 69591 Date: 9/12/02
Art Unit: 1621 Phone Number 308 45519 Serial Number: 10 661 617 10 664,123
Mail Box and Bldg/Room Location: (m) 7107 Results Format Preferred (circle): PAPER DISK E-MAIL

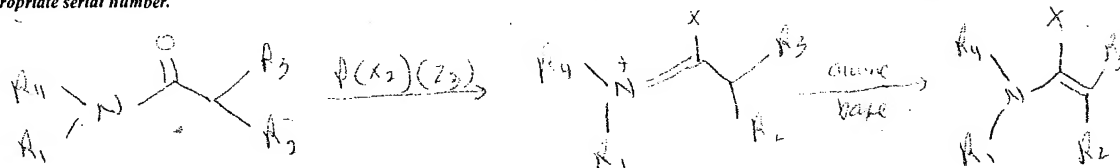
If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Alpha-haloenamine reagents
Inventors (please provide full names): Dennis P. Phillion

Earliest Priority Filing Date: 8/30/2001

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



See Dennis 1.64.
Also see various examples.

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Type of Search

NA Sequence (#) ...
AA Sequence (#) ...
Structure (#) ✓
Bibliographic ...
Litigation ...
Fulltext ...
Patent Family ...
Other ...

Vendors and cost where applicable

STN ✓
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Other (specify) ...

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(FILE 'HOME' ENTERED AT 06:57:08 ON 19 SEP 2002)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 06:57:32 ON 19 SEP 2002

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L1 30 S E3,E4,E6-E8
E US2002-061617/AP, PRN
E WO2002-US27953/AP, PRN
E WO2002-US25609/AP, PRN
E US2001-316151
E US2001-316151/AP, PRN
L2 0 S L1 AND HALOENAMINE
L3 16 S HALOENAMINE
L4 11 S L3 AND ALPHA
L5 606 S AMINE#/CW (L) ENAMINE
L6 240 S AMINE#/CW (L) HALO
L7 4 S L5 AND L6
L8 3 S L7 AND ALPHA
L9 13 S L4,L8
L10 5 S L3 NOT L9
L11 103 S HALO(S) ENAMINE
L12 154 S HALO(L) ENAMINE
L13 48 S L11,L12 AND ALPHA
L14 9 S L9 AND L13
L15 13 S L9,L14
L16 39 S L13 NOT L15
L17 4 S L16 AND L6,L5
L18 17 S L15,L17
L19 35 S L16 NOT L18
SEL DN AN 7 8 9 13 23 24
L20 6 S L19 AND E1-E18
L21 23 S L18,L20
L22 24 S ALPHA() (CHLOROENAMINE OR BROMOENAMINE OR FLUOROENAMINE OR IOD
L23 68 S ALPHA(S) (CHLORO OR BROMO OR FLUORO OR IODO) (S) ENAMINE
L24 41 S ALPHA(S) HALO? (S) ENAMINE
L25 17 S L21 AND L22-L24
L26 23 S L21,L25
L27 105 S L22-L24 NOT L26
L28 97 S L27 NOT L19
L29 44 S L28 AND (NEW REAGENT OR REACTIVE INTERMEDIATE OR SYNTHESIS OR
SEL DN AN 9 23 26 27 30 34 38 39 41 44
L30 10 S E19-E48 AND L29
L31 33 S L26,L30
E ENAMINE/CT
E E4+ALL
L32 1739 S E8
L33 156 S L32 (L) (HALO? OR CHLORO? OR BROMO? OR FLUORO? OR IODO? OR CH
L34 131 S L33 NOT L13-L31
L35 4 S L34 AND (PARTIALLY FLUORINATED OR BROMINATION OR VERY MILD CO
SEL DN AN 2-3
L36 2 S L35 AND E1-E6
L37 37 S L31,L35
L38 76 S L32 (L) ALPHA
L39 56 S L38 NOT L33-L37
L40 37 S L37 AND L1-L39
L41 37 S L40 AND ?ENAMINE?
L42 37 S L41 AND (HALO? OR CHLOR? OR BROM? OR FLUOR? OR IODO? OR IODI?
L43 35 S L42 AND ALPHA
L44 2 S L42 NOT L43
L45 20436 S TRIETHYLAMINE OR TRIETHYL AMINE OR TRI ETHYLAMINE OR TRI ETHY
L46 20889 S TERTIARY AMINE

E TERTIARY AMINE/CT
E E6+ALL
L47 5470 S E2

FILE 'REGISTRY' ENTERED AT 07:46:31 ON 19 SEP 2002
L48 1 S 121-44-8

FILE 'HCAPLUS' ENTERED AT 07:47:18 ON 19 SEP 2002
L49 17005 S L48
L50 148 S DIETHYLAMINOETHANE OR DIETHYLAMINO ETHANE OR DIETHYL ETHANAMI
L51 47070 S L45-L47,L49,L50
L52 1 S PENTAVAl?(L)PHOSPHOROUS(S) (HALIDE OR CHLORIDE OR BROMIDE OR I
L53 106 S PHOSPHOROUS() (PENTABROMIDE OR PENTACHLORIDE OR PENTAFLUORIDE
L54 3643 S PHOSPHOR?() (PENTABROMIDE OR PENTACHLORIDE OR PENTAFLUORIDE OR
L55 6 S PHOSPHOR? PENTAiodide

FILE 'REGISTRY' ENTERED AT 07:55:17 ON 19 SEP 2002
L56 4 S 10026-13-8 OR 7789-69-7 OR 7647-19-0 OR 66656-29-9
L57 840 S P/ELS AND (CL OR BR OR I OR F)/ELS NOT (C OR N OR S OR SI OR
L58 526 S L57 NOT (CCS OR RIS OR PMS OR MNS)/CI
L59 48 S L58 AND NR>=2
L60 478 S L58 NOT L59
L61 279 S L60 AND 1/NC
L62 215 S L61 AND 1/P
L63 124 S L62 NOT (TIS OR AYS)/CI
L64 119 S L63 NOT 37CL
L65 114 S L64 NOT SE/ELS
L66 113 S L65 NOT CA/ELS
L67 108 S L66 NOT B/ELS
L68 107 S L67 NOT MN/ELS
L69 100 S L68 NOT ((CD OR GE)/ELS OR 35CL)
L70 98 S L69 NOT (TA OR NB)/ELS
L71 93 S L70 NOT 32P
L72 83 S L71 NOT (36CL OR 33P OR 18F OR 35P OR 74BR OR 35CL OR P35CL?
L73 81 S L72 NOT (P79BR? OR 79BR)
L74 72 S L73 NOT (CLP OR BRP OR IP OR FP OR P81BR?)
L75 13 S L74 AND 6/ATC
L76 13 S L56,L75
L77 59 S L74 NOT L76

FILE 'HCAPLUS' ENTERED AT 08:09:17 ON 19 SEP 2002
L78 2781 S L76
L79 5810 S L77
L80 9904 S L78,L79,L52-L55
SEL RN L22
DEL SEL

FILE 'REGISTRY' ENTERED AT 08:10:53 ON 19 SEP 2002

FILE 'HCAPLUS' ENTERED AT 08:10:53 ON 19 SEP 2002
SET SMARTSELECT ON
L81 SEL L22 1- RN : 509 TERMS
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 08:10:54 ON 19 SEP 2002
L82 509 S L81
L83 198 S L82 AND (N AND (CL OR BR OR I OR F))/ELS
L84 STR
L85 50 S L84
L86 25524 S L84 FUL
L87 STR L84
L88 2480 S L87 FUL SUB=L86
SAV L88 KUMAR061/A

L89 STR L87
L90 10183 S L89 FUL SUB=L86
SAV L90 KUMAR061A/A
L91 2124 S L88 AND 1/NC
L92 356 S L88 NOT L91

FILE 'HCAPLUS' ENTERED AT 08:17:39 ON 19 SEP 2002

L93 1163 S L88
L94 41 S L93 AND L51
L95 43 S L93 AND L80
L96 5714 S L90
L97 34 S L83 AND L96
L98 1 S L94 AND L95 AND L96
L99 72 S L88/P AND L94,L95,L97
L100 26 S L99 AND (L51(L) (RACT OR RCT OR RGT OR CAT)/RL OR L90(L) (RACT
L101 16 S L100 AND L51
L102 64 S L93 AND L3-L6,L11,L12,L22-L24,L32-L34
L103 3 S L102 AND L80
L104 15 S L43 AND L93-L103,L45-L47,L49-L55,L78-L80
L105 35 S L43,L104
L106 59697 S ACETONITRILE
L107 113831 S TETRAHYDROFURAN
L108 7836 S 1 4 DIOXANE
L109 12138 S METHYLENECHLORIDE OR METHYLENE CHLORIDE
L110 39945 S CHLOROFORM
L111 10466 S 1 2 DICHLOROETHANE
L112 64 S 1 2 DICHLORO ETHANE
L113 127691 S TOLUENE
L114 245181 S BENZENE

FILE 'REGISTRY' ENTERED AT 08:33:43 ON 19 SEP 2002

L115 8 S 75-05-8 OR 109-99-9 OR 123-91-1 OR 75-09-2 OR 67-66-3 OR 71-4

FILE 'HCAPLUS' ENTERED AT 08:33:54 ON 19 SEP 2002

L116 0 S L104 AND L106-L114,L115
L117 9 S L1 AND L2-L47,L49-L55,L78-L80,L93-L114
L118 220 S PHARMACIA?/PA,CS AND L2-L47,L49-L55,L78-L80,L93-L114
L119 1 S L118 AND L93
L120 0 S L118 AND L3-L6,L11,L12,L22-L24,L32-L34

FILE 'REGISTRY' ENTERED AT 08:37:50 ON 19 SEP 2002

L121 1 S L88 AND C6H12CLN/MF
L122 4 S L88 AND C12H16CLN/MF AND 46.150.18/RID
L123 1 S L122 NOT BUTEN
L124 59 S (C11H16N2O4 OR C11H15CLN2O3)/MF AND NC4/ES AND 1/NR
L125 42 S L124 AND ESTER
L126 30 S L124 AND 16.136.9/RID
L127 19 S L125 AND L126
L128 5 S L127 AND 1 METHYL
L129 25 S L126 NOT L128
L130 3 S L129 AND 1 METHYL
L131 1 S 77716-11-1
L132 3 S L124 AND CL/ELS
L133 20 S C10H13CLO2SI/MF AND 46.150.18/RID
L134 1 S L133 AND BENZOIC ACID AND 2 CHLORO 6
L135 7 S C10H12CL2OSI/MF AND 46.150.18/RID AND 1/NR
L136 1 S L135 AND BENZOYL CHLORIDE
L137 101 S C7H6O3/MF AND 46.150.18/RID AND 1/NR
L138 28 S L137 AND 2 HYDROXY
L139 27 S L138 AND BENZOIC
E BENZOIC ACID, 2-HYDROXY-/CN
L140 1 S E3
L141 67 S C7H5CLO2/MF AND 46.150.18/RID AND 1/NR

L142 7 S L141 AND 2 HYDROXY
L143 1 S 1441-87-8
L144 260 S C8H8O3/MF AND 46.150.18/RID AND 1/NR
L145 6 S L144 AND 2 HYDROXY AND METHYL ESTER
L146 1 S 119-36-8
L147 26 S L137 AND 4 HYDROXY AND BENZOIC
L148 1 S 99-96-7
L149 4 S L141 AND 4 HYDROXY
L150 1 S 28141-24-4
L151 9 S L144 AND 4 HYDROXY AND METHYL ESTER
L152 1 S 99-76-3
L153 378 S C8H9NO2/MF AND 46.150.18/RID AND 1/NR
L154 47 S L153 AND 4 HYDROXY
L155 1 S L154 AND BENZAMIDE AND N METHYL
L156 16 S C11H16CLNOSI/MF AND 46.150.18/RID AND 1/NR
L157 2 S L156 AND BENZAMIDE
L158 1 S 150108-45-5
L159 69 S C7H5NO4/MF AND 46.150.18/RID AND 1/NR
L160 12 S L159 AND 2 NITRO
L161 7 S L160 AND BENZOIC
L162 1 S 552-16-9
L163 12 S C7H4CLNO2/MF AND 46.150.18/RID AND 1/NR
L164 28 S C7H4CLNO3/MF AND 46.150.18/RID AND 1/NR
L165 1 S L164 AND BENZOYL CHLORIDE AND 2 NITRO
L166 169 S C8H7NO4/MF AND 46.150.18/RID AND 1/NR
L167 32 S L166 AND 2 NITRO
L168 7 S L167 AND BENZOIC ACID
L169 1 S 606-27-9
L170 198 S C8H8N2O3/MF AND 46.150.18/RID AND 1/NR
L171 32 S L170 AND 2 NITRO
L172 1 S L171 AND BENZAMIDE AND N METHYL

FILE 'HCAPLUS' ENTERED AT 09:26:12 ON 19 SEP 2002

L173 71 S L121
L174 0 S L131 AND L121

FILE 'REGISTRY' ENTERED AT 09:26:45 ON 19 SEP 2002

L175 45 S NCNC2/ES AND C10H15N3O4/MF AND 1/NR
L176 10 S L175 AND 1 METHYL
L177 1 S 128293-64-1
L178 0 S NCNC2/ES AND C10H14CLN3O3/MF AND 1/NR

FILE 'HCAPLUS' ENTERED AT 09:30:03 ON 19 SEP 2002

L179 0 S L177 AND L173
L180 1 S L123
L181 0 S (L134, L136, L158, L140, L143, L146, L148, L150, L152, L155, L162, L165,
L182 1 S L134 AND L136, L158
L183 1 S L136 AND L158
L184 1 S L182, L183
L185 529 S L140 AND L143, L146
L186 13 S L143 AND L146
L187 8 S L185 AND L186
L188 0 S L146/P AND L187
L189 554 S L148 AND (L150, L152, L155)
L190 3 S L150 AND L152, L155
L191 2 S L189 AND L190
L192 0 S (L152/P OR L155/P) AND L191
L193 59 S L162 AND L165, L169, L172
L194 2 S L165 AND L169, L172
L195 0 S L193 AND L194
L196 0 S L1 AND L173, L123
L197 2 S L1 AND L131, L177, L134, L136, L158, L140, L143, L146, L148, L150, L152
L198 2 S L184, L197

L199 37 S L105,L198
L200 0 S N 1 CHLORO 2 METHYLPROP 1 ENYL N METHYL AMINOMETHYL?
L201 10 S CHLORO(L)METHYLPROP?(L)?AMINOMETHYL?
L202 0 S L180 AND ?STYREN?

=> fil hcaplus

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FILE COVERS 1907 - 19 Sep 2002 VOL 137 ISS 12

FILE LAST UPDATED: 18 Sep 2002 (20020918/ED)

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=> d l199 all tot

L199 ANSWER 1 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 2001:799119 HCAPLUS

DN 136:199946

TI **.alpha.-Bromination** of .beta.-enamino compounds using K-10

AU Braibante, Mara E. F.; Braibante, Hugo T. S.; Rosso, Giovanni B.; Da Roza, Juliano K.

CS Departamento de Quimica, Universidade Federal de Santa Maria, Santa Maria, 97105-900, Brazil

SO Synthesis (2001), (13), 1935-1937

CODEN: SYNTBF; ISSN: 0039-7881

PB Georg Thieme Verlag

DT Journal

LA English

CC 24-5 (Alicyclic Compounds)

OS CASREACT 136:199946

AB **.alpha.-Bromo-3-amino-5,5-dimethylcyclohex-2-en-1-ones**

and **.alpha.-bromo-.beta.-enamino** compds.

MeC(NH2):CBrCOR (R = Me, OEt) were conveniently prepd. using NBS supported on montmorillonite (K-10). Other reaction conditions such as di-tert-Bu peroxide/NBS/CCl4, and Br2/CH2Cl2 were also studied for 3-amino-5,5-dimethylcyclohex-2-en-1-ones resulting in a mixt. of mono and di-brominated compds.

ST montmorillonite catalyst regioselective **bromination enamine**

IT **Bromination**

Bromination catalysts
Regiochemistry

(.alpha.-bromination of .beta.-enamino compds.
using K-10)

IT Enamines

RL: RCT (Reactant); RACT (Reactant or reagent)

(.alpha.-bromination of .beta.-enamino compds.
using K-10)

IT 1318-93-0, Montmorillonite K-10, uses

RL: CAT (Catalyst use); USES (Uses)

(.alpha.-bromination of .beta.-enamino compds.
using K-10)

IT 701-58-6 873-95-0, 3-Amino-5,5-dimethylcyclohex-2-en-1-one 889-31-6
1118-66-7 7318-00-5 15255-66-0 18940-21-1 55800-10-7 80555-73-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(.alpha.-bromination of .beta.-enamino compds.
using K-10)

IT 51924-66-4P 51924-68-6P 52265-03-9P 102689-02-1P 159423-68-4P
401511-96-4P 401511-97-5P 401511-98-6P 401511-99-7P 401512-00-3P
401512-01-4P 401512-02-5P 401512-03-6P 401512-04-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(.alpha.-bromination of .beta.-enamino compds.
using K-10)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Alberola, A; Synth Commun 1986, V16, P1161 HCAPLUS
- (2) Braibante, M; J Heterocycl Chem 1997, V34, P1453
- (3) Braibante, M; J Heterocycl Chem 1998, V35, P189
- (4) Braibante, M; Synthesis 1994, P898 HCAPLUS
- (5) Braibante, M; Synthesis 1998, P1019
- (6) Jirkovsky, I; Can J Chem 1974, P55 HCAPLUS
- (7) Pitchumani, K; Tetrahedron 1997, V53, P2581
- (8) Rosso, G; M Sc Dissertation, Universidade Federal de Santa Maria 2000

L199 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 2001:773362 HCAPLUS

DN 136:263126

TI Syntheses and reactions of .alpha.-

benzotriazolylenamines: stable analogs of .alpha.-
chloroenamines

AU Katritzky, Alan R.; Nichols, Daniel A.; Voronkov, Michael V.

CS Center for Heterocyclic Compounds, Dept. Chem., Univ. Florida,
Gainesville, FL, 32611-7200, USA

SO ARKIVOC [online computer file] (2000), 1(5), 667-683

CODEN: AKVCFI

URL: <http://www.arkat.org/arkat/journal/Issue5/ms0065/ms0065.pdf>

PB ARKAT Foundation

DT Journal; (online computer file)

LA English

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

AB Synthetic routes to and utility of .alpha.-

benzotriazolylenamines have been explored. .alpha.-

Benzotriazolylenamines were successfully synthesized (i) from
N-(trans-buten-1-yl)-N-methylaniline (2) by reaction with 1-chloro
-1H-1,2,3-benzotriazole, followed by base induced elimination of HCl and
(ii) from amides using benzotriazole, POCl₃ and NEt₃ in CH₃CN. The
utility of the products as stable alternatives to .alpha.-
haloenamines was demonstrated by the successful reaction of
N-[1-(2H-1,2,3-benzotriazol-2-yl)-2-methylprop-1-enyl]-N-methylaniline
with phenylethynylzinc **chloride** to form N-methyl-N-[2-methyl-1-
(2-phenylethynyl)-1-propenyl]aniline.

ST **benzotriazolylenamine** prepn reaction

IT 103-69-5 122-39-4, reactions 142-62-1, Hexanoic acid, reactions

6738-06-3, Phenylethynylmagnesium **bromide** 21050-95-3

40669-47-4 42883-79-4 55577-65-6 63017-96-9 144691-18-9

405103-81-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. and reactions of .alpha.-

benzotriazolylenamines)

IT 305851-38-1P 305851-39-2P 305861-36-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(prepn. and reactions of .alpha.-

benzotriazolylenamines)

IT 305861-35-2P 305861-37-4P 305861-38-5P 405103-82-4P 405103-83-5P

405103-84-6P 405103-85-7P 405103-86-8P 405103-87-9P 405103-88-0P

405103-89-1P 405103-90-4P 405103-91-5P 405103-92-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and reactions of .alpha.-

benzotriazolylenamines)

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Barluenga, J; J Chem Soc, Perkin Trans 1 1980, P2732 HCAPLUS
- (2) Bordwell, F; J Org Chem 1991, V56, P4218 HCAPLUS
- (3) Brown, H; J Am Chem Soc 1961, V83, P4549 HCAPLUS
- (4) Carlson, R; Acta Chem Scand Ser B 1984, V38, P49
- (5) Chan, Y; Organic Syntheses 1973, V53, P48 HCAPLUS
- (6) Da Costa, R; J Am Chem Soc 1979, V101, P4381 HCAPLUS
- (7) Devos, A; J Chem Soc, Chem Commun 1979, P1180 HCAPLUS
- (8) Dietliker, K; Helv Chim Acta 1983, V66, P262 HCAPLUS
- (9) Ernst, B; Tetrahedron Lett 1989, V30, P3081 HCAPLUS
- (10) Foti, C; J Org Chem 1995, V60, P2656 HCAPLUS
- (11) Fujisawa, T; Tetrahedron Lett 1983, V24, P5745 HCAPLUS
- (12) Fujisawa, T; Tetrahedron Lett 1984, V25, P4007 HCAPLUS
- (13) Ghosez, L; Angew Chem, Int Ed 1969, V8, P454 HCAPLUS
- (14) Ghosez, L; Angew Chem, Int Ed 1972, V11, P852 HCAPLUS
- (15) Ghosez, L; Tetrahedron 1998, V54, P9207 HCAPLUS
- (16) Haveaux, B; Organic Syntheses 1988, V6, P282
- (17) Haynes, L; Enamines: Synthesis, Structure and Reactions 1988
- (18) Heine, H; Synthesis 1981, P706 HCAPLUS
- (19) Hickmott, P; Tetrahedron 1982, V38, P1975 HCAPLUS
- (20) Hoornaert, C; Angew Chem, Int Ed 1975, V14, P569
- (21) Human, J; Nat 1946, V158, P877 HCAPLUS
- (22) Jiang, J; J Am Chem Soc 1999, V121, P593 HCAPLUS
- (23) Katritzky, A; Chem Ber 1990, V123, P1545 HCAPLUS
- (24) Katritzky, A; Chem Rev 1998, V98, P409 HCAPLUS
- (25) Katritzky, A; Heterocycles 1995, V41, P131 HCAPLUS
- (26) Katritzky, A; J Chem Soc, Perkin Trans 1 1989, P225 HCAPLUS
- (27) Katritzky, A; Tetrahedron 1990, V46, P8153 HCAPLUS
- (28) Khanna, I; J Org Chem 1995, V60, P960 HCAPLUS
- (29) Luker, T; J Org Chem 1997, V62, P3592 HCAPLUS
- (30) Luker, T; J Org Chem 1997, V62, P8131 HCAPLUS
- (31) Munyemana, F; Tetrahedron Lett 1989, V30, P3077 HCAPLUS
- (32) Rees, C; J Chem Soc, Chem Commun 1969, P1474 HCAPLUS
- (33) Rens, M; Tetrahedron Lett 1970, P3765 HCAPLUS
- (34) Revankar, G; J Heterocycl Chem 1968, V5, P785 HCAPLUS
- (35) Ried, W; Chem Ber 1965, V98, P3142 HCAPLUS
- (36) Riviere, M; Bull Soc Chim Fr 1968, P4430 HCAPLUS
- (37) Rogalska, E; J Org Chem 1984, V49, P1397 HCAPLUS
- (38) Villalgorido, J; Helv Chim Acta 1995, V78, P1983 HCAPLUS
- (39) von Braun, J; Ber Dtsch Chem Ges 1929, V62, P409
- (40) von Braun, J; Chem Ber 1919, V52, P2261
- (41) Wedler, C; Liebigs Ann 1996, V6, P881
- (42) Wiaux-Zamar, C; Angew Chem, Int Ed 1976, V15, P371
- (43) Yang, C; Synlett 1997, V7, P812

DN 132:334206

TI Synthesis of 1-dialkylamino- and 1- and 2-alkoxyenynes by Pd-catalyzed cross-coupling of 1-**haloenamines** and 1- and 2-mono-, 2,2-di-, and 1,2,2-tribromoalkenyl alkyl ethers with terminal alkynes

AU Kazankova, M. A.; Trostyanskaya, I. G.; Lutsenko, S. V.; Efimova, I. V.; Beletskaya, I. P.

CS Faculty of Chemistry, Moscow State University, Moscow, 119899, Russia

SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1999), 35(9), 1273-1277
CODEN: RJOCEQ; ISSN: 1070-4280

PB MAIK Nauka/Interperiodica Publishing

DT Journal

LA English

CC 23-9 (Aliphatic Compounds)
Section cross-reference(s): 25

OS CASREACT 132:334206

AB A new procedure was developed for stereoselective synthesis of new 2-dialkylaminoenynes, 1- and 2-alkoxyenynes, and 1-alkoxyenediynes by Pd-catalyzed cross-coupling of **chloroenamines** and mono-, tri-, and dibromoalkenyl alkyl ethers with terminal alkynes. The reactions of 1,2,2-tribromoethenyl alkyl ethers involve replacement of **bromine** in the **.alpha.**-position with respect to the alkoxy group.

ST enyne dialkylamino alkoxy prepn; palladium coupling **haloenamine bromoalkenyl** ether alkyne

IT Cross-coupling reaction
Cross-coupling reaction catalysts
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT Alkenynes
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT Eenediynes
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd.; palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT 7681-65-4, Cuprous **iodide** 13965-03-2,
Dichlorobis(triphenylphosphine)palladium 14221-01-3,
Tetrakis(triphenylphosphine)palladium
RL: CAT (Catalyst use); USES (Uses)
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT 536-74-3, Ethynylbenzene 627-41-8, Methyl propargyl ether 917-92-0,
tert-Butylacetylene 1066-54-2, (Trimethylsilyl)acetylene 7223-38-3,
N,N-Dimethylpropargylamine 35920-24-2 100704-20-9
189686-76-8 220580-64-3 233764-81-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

IT 267889-55-4P 267889-56-5P 267889-57-6P 267889-58-7P 267889-59-8P
267889-60-1P 267889-61-2P 267889-62-3P 267889-63-4P 267889-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-catalyzed cross-coupling of alkynes with **chloroenamine** and with alkyl **bromoalkenyl** ethers)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Alami, L; Tetrahedron Lett 1991, V32, P6109
- (2) Anderson, C; J Org Chem 1989, V54(7), P1502
- (3) Brunner, M; Synlett 1994, P627 HCAPLUS
- (4) Coulson, D; Inorg Chem 1972, V13, P121
- (5) Efimova, I; Russ J Org Chem 1995, V31(3), P296
- (6) Franck-Neumann, M; Synlett 1994, P657 HCAPLUS
- (7) Ghosez, L; CH 681623 1993 HCAPLUS
- (8) Hoornert, C; Angew Chem, Int Ed Engl 1975, V14, P569
- (9) Iguchi, K; J Org Chem 1993, V58(21), P5690 HCAPLUS
- (10) Paquett, L; J Org Chem 1990, V55, P2443
- (11) Rossi, R; Tetrahedron 1982, V38, P631 HCAPLUS
- (12) Sonogachira, R; Tetrahedron Lett 1975, V16, P4467
- (13) Trakarruk, W; Organometallics 1994, V13, P3914
- (14) Trostyanskaya, I; Russ J Org Chem 1996, V32(7), P946
- (15) Wong, T; J Org Chem 1994, V59, P5527 HCAPLUS

L199 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1998:480680 HCAPLUS

DN 129:216202

TI A general and practical method of synthesis of 2-disubstituted 1-chloro enamines and 1-bromo enamines

AU Ghosez, Leon; George-Koch, Isabelle; Patiny, Luc; Houtekie, Marc; Bovy, Philippe; Nshimyumukiza, Prosper; Phan, Thao

CS Laboratoire de Chimie organique de Synthe, Universite catholique de Louvain, Louvain-la-Neuve, B - 1348, Belg.

SO Tetrahedron (1998), 54(31), 9207-9222

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

CC 21-2 (General Organic Chemistry)

OS CASREACT 129:216202

AB Disubstituted-.alpha.-chloroenamines are useful synthetic intermediates which had earlier been prepd. by the reaction of tertiary amides with phosgene. The toxicity of the latter led us to systematically investigate new synthetic routes towards .alpha.-chloro enamines and .alpha.-bromo enamines. The reactions of various halogenating agents (SOCl₂, diphosgene, triphosgene, OPCl₃, OPBr₃) with tertiary amides followed by the addn. of triethylamine have been studied. Thionyl chloride was found unsuitable for the prepn. of .alpha.-chloroenamines. Of the other halogenating agents, OPCl₃ and OPBr₃ were found the most practical. The generality of the method is illustrated by the synthesis of fifteen .alpha.-chloroenamines and six .alpha.-bromo enamines.

ST bromo enamine prepn; chloro enamine prepn

IT Enamines

RL: SPN (Synthetic preparation); PREP (Preparation)

(.alpha.-halo; prepn. of chloro enamines and bromo enamines)

IT 62-53-3, Benzenamine, reactions 79-30-1, 2-Methylpropanoyl chloride 100-61-8, reactions 108-18-9, Diisopropylamine 110-85-0, Piperazine, reactions 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 124-40-3, Dimethylamine, reactions 872-50-4, reactions 957-51-7, N,N-Dimethyldiphenylacetamide 2556-73-2, N-Methylcaprolactam 2719-27-9, Cyclohexanecarbonyl chloride 3282-30-2, Pivaloyl chloride 23356-96-9, L-Prolinol 35660-94-7, Tigloyl chloride 134860-30-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of chloro enamines and bromo

- enamines)**
- IT 6282-98-0P 17566-51-7P 18071-39-1P 18940-58-4P 19597-07-0P
 21678-37-5P 32223-06-6P 33931-47-4P 55577-65-6P 55917-05-0P
 143726-38-9P 212518-24-6P 212518-25-7P 212518-26-8P 212518-27-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of **chloro enamines** and **bromo enamines**)
- IT 26189-59-3P 58933-80-5P 58933-81-6P
 60180-60-1P 65785-45-7P 66206-72-2P
 73630-93-0P 75115-55-8P 87443-04-7P
 116437-56-0P 149554-70-1P 201679-72-3P
 201679-73-4P 201679-74-5P 201679-78-9P
 201679-79-0P 201679-80-3P 201679-81-4P
 201679-82-5P 212518-28-0P 212518-29-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of **chloro enamines** and **bromo enamines**)
- L199 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2002 ACS
 AN 1998:804 HCAPLUS
 DN 128:114663
 TI Electron ionization and CID mass spectra of **.alpha.-halo enamines**
 AU de Hoffmann, E.; George-Koch, I.; Ghosez, L.
 CS Dep. of Chem., Univ. Catholique de Louvain, Louvain-la-Neuve, 1348, Belg.
 SO Bulletin des Societes Chimiques Belges (1997), 106(7-8), 475-479
 CODEN: BSCBAG; ISSN: 0037-9646
 PB Bulletin des Societes Chimiques Belges
 DT Journal
 LA English
 CC 22-8 (Physical Organic Chemistry)
 AB Fragmentations of ions obtained by electron-impact ionization of 25
chloro- and bromoenamines were studied by low
 collision-energy tandem mass spectrometry. For most compds., the main
 fragmentation pathways involved (a) loss of an **halogen** atom, (b)
 loss of an alkyl group linked to the N atom, and (c) loss of an alkyl
 fragment from the **.beta.-position**. Some structural features were found to
 induce specific fragmentation pathways. Thus, when the entire
enamine function is part of a 5-membered ring, loss of an H atom
 was obsd. as a result of a stereoelectronic effect. The presence of a
 vinyl group at the **.beta.-position** gave fragments contg. a pyridine ring.
- ST **halo enamine** mass spectra; fragmentation **halo enamine** mechanism
- IT Collision-induced dissociation
 Fragmentation reaction
 Mass spectra
 Stereoelectronic effect
 (fragmentation mechanisms in electron-ionization and CID mass spectra
 of **.alpha.-halo enamines**)
- IT **Enamines**
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (**.alpha.-halo-**; fragmentation mechanisms in
 electron-ionization and CID mass spectra of **.alpha.-halo enamines**)
- IT 26189-59-3 35920-24-2 58933-80-5
 58933-81-6 60180-60-1 65785-45-7
 66206-72-2 73630-93-0 75115-55-8 87443-04-7
 116437-56-0 149554-70-1 201679-72-3
 201679-73-4 201679-74-5 201679-75-6
 201679-76-7 201679-77-8 201679-78-9
 201679-79-0 201679-80-3 201679-81-4
 201679-82-5 201679-83-6 201679-84-7

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(fragmentation mechanisms in electron-ionization and CID mass spectra
of **.alpha.-halo enamines**)

L199 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1997:403882 HCAPLUS

DN 127:121576

TI Introduction of **bromine** and **chlorine** substituents in
medium ring ethers and lactones

AU Bendall, Justin G.; Payne, Andrew N.; Screen, Thomas E. O.; Holmes, Andrew
B.

CS Univ. Chem. Lab., Cambridge, CB2 1EW, UK

SO Chemical Communications (Cambridge) (1997), (11), 1067-1068

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

DT Journal

LA English

CC 26-1 (Biomolecules and Their Synthetic Analogs)

OS CASREACT 127:121576

AB A convenient prepn. of **.alpha.-halo enamines**

Me₂NC(X)=CMe₂ (X = Br, Cl) using oxalyl halides is described together with
applications of these reagents in the **halogenation** of
.beta.-hydroxy cyclic ethers and lactones.

ST **enamine alpha halo** prepn; medium ring ether

lactone **halogenation**

IT Ethers, preparation

Lactones

RL: SPN (Synthetic preparation); PREP (Preparation)

(medium ring; mild synthesis of **.alpha.-halo**

enamine for **halogenating** medium ring ethers and

lactones)

IT **Halogenation**

(mild synthesis of **.alpha.-halo enamine**

for **halogenating** medium ring ethers and lactones)

IT 453-20-3 590-67-0 2216-51-5, (-)-Menthol 21678-37-5 84214-06-2

97514-97-1 192719-10-1 192719-13-4 192719-17-8 192766-39-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(mild synthesis of **.alpha.-halo enamine**

for **halogenating** medium ring ethers and lactones)

IT 26189-59-3P 73630-93-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(mild synthesis of **.alpha.-halo enamine**

for **halogenating** medium ring ethers and lactones)

IT 931-77-1P 931-78-2P 13371-12-5P 19311-37-6P 19311-38-7P

87161-57-7P 192719-11-2P 192719-12-3P 192719-14-5P 192719-15-6P

192719-16-7P 192719-18-9P 192719-19-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(mild synthesis of **.alpha.-halo enamine**

for **halogenating** medium ring ethers and lactones)

L199 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1996:737347 HCAPLUS

DN 126:103659

TI **Halogenation** of 1-trifluoromethyl **enamines**: A new and
efficient **synthesis** of **.alpha.-bromo-** and
.alpha.-iodo-trifluoromethyl ketones

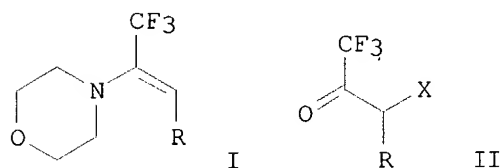
AU Begue, Jean-Pierre; Bonnet-Delpon, Daniele; Bouvet, Denis; Rock, Michael
H.

CS BioCIS-CNRS, Centre d'Etudes Pharmaceutiques, Rue J.B. Clement, F-92296,
Chatenay-Malabry, Fr.

SO Journal of Fluorine Chemistry (1996), 80(1), 17-20

CODEN: JFLCAR; ISSN: 0022-1139

PB Elsevier
 DT Journal
 LA English
 CC 21-2 (General Organic Chemistry)
 Section cross-reference(s): 27
 OS CASREACT 126:103659
 GI



- AB Treatment of the 1-trifluoromethyl **enamines** I (R = alkyl, phenyl) with **bromine** or **iodine** resulted in the formation of the corresponding iminium salts. Treatment of any of these salts with methanol resulted in the formation of the corresponding **alpha.-haloalkyl** trifluoromethyl ketones II (same R; X = chloro, iodo).
- ST **fluoromethyl enamine halogenation**; ketone
 trifluoromethyl **haloalkyl** prepn; alkanone trifluoro prepn
- IT **Halogenation**
 (prepn. of trifluoromethyl ketones by **halogenation** of (trifluoromethyl)**enamines**)
- IT **Enamines**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (trifluoromethyl; prepn. of trifluoromethyl ketones by **halogenation** of (trifluoromethyl)**enamines**)
- IT Ketones, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (trifluoromethyl; prepn. of trifluoromethyl ketones by **halogenation** of (trifluoromethyl)**enamines**)
- IT 7553-56-2, **Iodine**, reactions 7726-95-6, **Bromine**, reactions 123007-80-7 186001-39-8 186001-40-1 186001-41-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of trifluoromethyl ketones by **halogenation** of (trifluoromethyl)**enamines**)
- IT 186001-46-7P 186001-47-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of trifluoromethyl ketones by **halogenation** of (trifluoromethyl)**enamines**)
- IT 395-15-3P 122977-77-9P 122977-78-0P 122977-79-1P 186001-42-3P
 186001-43-4P 186001-44-5P 186001-45-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of trifluoromethyl ketones by **halogenation** of (trifluoromethyl)**enamines**)

L199 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1996:108957 HCAPLUS

DN 124:288383

TI **Bromination** of secondary and tertiary **enamines**

AU Lyubchanskaya, V. M.; Mukhanova, T. I.; Alekseeva, L. M.; Granik, V. G.

CS TsKhLS, VNIKhFI, Moscow, Russia

SO Khimiko-Farmatsevticheskii Zhurnal (1995), 29(11), 37-40

CODEN: KHFZAN; ISSN: 0023-1134

PB Meditsina

DT Journal

LA Russian
CC 21-2 (General Organic Chemistry)
AB Secondary and tertiary **enamines** having an **.alpha.-Me** group and a H atom at the **.beta.** position were **brominated** by Br₂ or N-**bromosuccinimide**. The secondary **enamines** were **brominated** at the **.beta.** position; the tertiary **enamines** were **brominated** on the **.alpha.-Me** group. Further reactions of the **.alpha.-(bromomethyl)** tertiary **enamines** with amines and with CN⁻ were studied.
ST **bromination enamine** regiochem; cyano **enamine** prepn; amino **enamine** prepn
IT Regiochemistry
(of **bromination** of **enamines**)
IT **Bromination**
(regiochem. of **bromination** of **enamines**)
IT **Enamines**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regiochem. of **bromination** of **enamines**)
IT 16195-93-0 18594-93-9 20771-70-4 20771-77-1 25236-38-8
34523-87-0 62875-03-0 175544-34-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(regiochem. of **bromination** of **enamines**)
IT 175544-40-8P 175544-42-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regiochem. of **bromination** of **enamines**)
IT **175544-35-1P 175544-36-2P 175544-37-3P 175544-38-4P**
175544-39-5P 175544-41-9P 175544-43-1P 175544-44-2P 175544-45-3P
175544-46-4P 175544-47-5P 175544-48-6P 175544-49-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regiochem. of **bromination** of **enamines**)

L199 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1995:983031 HCAPLUS
DN 124:145558
TI Metalation Chemistry of N-Ethyl-N-(1-methoxy-2,2-dimethylpropyl)benzamides. A New Protective Group for Secondary Amides
AU **Phillion, Dennis P.; Walker, Daniel M.**
CS Ceregen A Unit, Monsanto Co., St. Louis, MO, 63167, USA
SO Journal of Organic Chemistry (1995), 60(26), 8417-20
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 124:145558
AB The synthesis of N-ethyl-N-(1-methoxy-2,2-dimethylpropyl)benzamides and their metalation with s-BuLi or LTMP (lithium 2,2,6,6-tetramethylpiperidide) is described. These protected N-ethylbenzamides are synthesized in excellent yields through the addn. of N-ethyltrimethylacetaldehyde imine to a benzoyl chloride, followed by reaction of the intermediate **.alpha.-chloroamide** with methanol and triethylamine. Hydrolysis to their corresponding N-ethylbenzamides is achieved under mild acid conditions with aq. HCl in dioxane. N-ethyl-N-(1-methyl-2,2-dimethylpropyl)benzamide ortho-lithio deriv. was stable at room temp. yet reacted with electrophiles at -78.degree.. The metalation and reaction of other N-ethyl-N-(1-methoxy-2,2-dimethylpropyl)benzamides is also described.
ST benzamide protection methoxydimethylpropyl prepn reaction; ortho lithiation protected ethylbenzamide
IT Metalation
Protective groups

(prepn. of (methoxydimethylpropyl)-protected ethylbenzamides and their ortho metalation chem.)

IT 68-12-2, Dmf, reactions 75-04-7, Ethylamine, reactions 624-73-7, 1,2-Diiodoethane 630-19-3, Trimethylacetaldehyde 2949-92-0
150079-25-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of (methoxydimethylpropyl)-protected ethylbenzamides and their ortho metalation chem.)

IT 52135-87-2P 150078-39-0P 150079-68-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of (methoxydimethylpropyl)-protected ethylbenzamides and their ortho metalation chem.)

IT 52369-57-0P 150078-25-4P 150078-61-8P 150078-69-6P 150078-77-6P 150079-83-7P 173204-22-3P 173204-23-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of (methoxydimethylpropyl)-protected ethylbenzamides and their ortho metalation chem.)

L199 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1993:560256 HCAPLUS
DN 119:160256
TI Preparation of heterocyclic and aromatic compounds as fungicides for the control of take-all disease of plants
IN **Phillion, Dennis Paul**; Braccolino, Diane Susan; Graneto, Matthew James; Phillips, Wendell Gary; Van Sant, Karey Alan; Walker, Daniel Mark; Wong, Sai Chi
PA Monsanto Co., USA
SO Eur. Pat. Appl., 78 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM A01N055-00
ICS A01N037-18; A01N055-02; A01N037-40; C07F007-08; C07F007-22; C07F007-30; C07C233-65; C07C317-44; A01N055-04; A01N037-44; C07C235-60; C07C323-62; C07C233-69; C07C237-30; C07C233-66
CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5, 25
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| EP 538231 | A1 | 19930421 | EP 1992-870168 | 19921016 |
| EP 538231 | B1 | 20010613 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| WO 9307751 | A1 | 19930429 | WO 1992-US8633 | 19921009 |
| W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KR, LK, MG, MN, MW, NO, PL, RO, RU, SD | | | | |
| RW: BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG | | | | |
| AU 9228093 | A1 | 19930521 | AU 1992-28093 | 19921009 |
| AU 664392 | B2 | 19951116 | | |
| HU 66952 | A2 | 19950130 | HU 1994-1110 | 19921009 |
| HU 219131 | B | 20010228 | | |
| PL 170837 | B1 | 19970131 | PL 1992-303097 | 19921009 |
| CZ 290470 | B6 | 20020717 | CZ 1994-887 | 19921009 |
| LV 10020 | B | 19950220 | LV 1992-154 | 19921015 |
| LT 3276 | B | 19950525 | LT 1992-193 | 19921015 |
| ZA 9208024 | A | 19930827 | ZA 1992-8024 | 19921016 |
| EP 1088481 | A2 | 20010404 | EP 2000-124212 | 19921016 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE | | | | |
| ES 2159507 | T3 | 20011016 | ES 1992-870168 | 19921016 |
| CN 1085221 | A | 19940413 | CN 1993-100002 | 19930102 |
| CN 1043835 | B | 19990630 | | |
| US 5498630 | A | 19960312 | US 1994-340573 | 19941116 |

| | | | | |
|----------------------|---|----------|----------------|----------|
| US 5693667 | A | 19971202 | US 1994-365391 | 19941228 |
| US 5705513 | A | 19980106 | US 1994-365619 | 19941228 |
| US 5849723 | A | 19981215 | US 1994-365382 | 19941228 |
| US 5834447 | A | 19981110 | US 1995-569273 | 19951208 |
| US 5811411 | A | 19980922 | US 1996-754920 | 19961122 |
| US 6028101 | A | 20000222 | US 1997-908201 | 19970807 |
| US 5998466 | A | 19991207 | US 1998-31007 | 19980226 |
| US 36562 | E | 20000208 | US 1998-41113 | 19980311 |
| CN 1221745 | A | 19990707 | CN 1998-116778 | 19980801 |
| CN 1221746 | A | 19990707 | CN 1998-116779 | 19980801 |
| CN 1225364 | A | 19990811 | CN 1998-116864 | 19980801 |
| CN 1225365 | A | 19990811 | CN 1998-116865 | 19980801 |
| US 6248894 | B1 | 20010619 | US 1998-161842 | 19980928 |
| US 6252078 | B1 | 20010626 | US 1998-162032 | 19980928 |
| US 6133252 | A | 20001017 | US 1998-186176 | 19981104 |
| US 6166057 | A | 20001226 | US 1998-185938 | 19981104 |
| US 6410558 | B1 | 20020625 | US 2000-722829 | 20001127 |
| US 2001046975 | A1 | 20011129 | US 2001-851836 | 20010509 |
| PRAI US 1991-780683 | A | 19911018 | | |
| US 1992-951997 | A | 19921002 | | |
| WO 1992-US8633 | A | 19921009 | | |
| EP 1992-870168 | A3 | 19921016 | | |
| US 1994-238182 | A3 | 19940504 | | |
| US 1994-340573 | A3 | 19941116 | | |
| US 1994-365382 | A3 | 19941228 | | |
| US 1994-365391 | A3 | 19941228 | | |
| US 1995-569273 | A3 | 19951208 | | |
| US 1996-754920 | A3 | 19961122 | | |
| US 1998-162032 | A3 | 19980928 | | |
| OS MARPAT 119:160256 | | | | |
| AB | Derivs. of benzene, pyridine, thiophene, furan, pyrrole, pyrazole, thiazole, and isothiazole are claimed as fungicides for the control of take-all disease of plants. Substituents on these arom. ring systems include amides, thioamides, S-alkyl thiocarboxylates, imino derivs., various organosilyl, organogermyl, or organostannyl derivs., aryl derivs., and other org. groups. Preparative examples include benzamide derivs., benzenecarbothioate derivs., and pyridinecarboxamides, among many others. The compds. (285 examples) were effective at 0.1-10 ppm for control of Gaemannomyces graminis var. tritici in vitro, and many of these compds. showed 100% control of the fungi in vivo on Bergen and Anza varieties of wheat. Application of the fungicide to the seed prior to planting is the preferred method of treatment for the disease. | | | |
| ST | fungicide heterocyclic arom prepn; wheat take all disease fungicide | | | |
| IT | Fungicides and Fungistats (arom. and heterocyclic compds., for control of take-all disease in plants) | | | |
| IT | Aromatic compounds Heterocyclic compounds RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as fungicides for control of take-all disease) | | | |
| IT | Wheat (disease, take-all, control of, arom. and heterocyclic compds. as fungicides for) | | | |
| IT | 6196-85-6, 1-Chloro-1-methylcyclopentane 10523-97-4, 1-Chloro-1-methylcyclobutane RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation by, of benzamide) | | | |
| IT | 1066-54-2, Trimethylsilylacetylene RL: RCT (Reactant); RACT (Reactant or reagent) (alkynylation by, of benzamide) | | | |
| IT | 765-30-0, Cyclopropylamine 2450-71-7, Propargylamine RL: RCT (Reactant); RACT (Reactant or reagent) (amidation by, of benzoyl chloride deriv.) | | | |

- IT 107-11-9, 2-Propen-1-amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of thiophenecarboxylic acid)
- IT 89-75-8, 2,4-Dichlorobenzoyl chloride 1710-98-1, 4-tert-Butylbenzoyl chloride 2905-61-5, 2,5-Dichlorobenzoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)
- IT 106-93-4, Ethylene dibromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination by, of (trimethylsilyl)benzamide)
- IT 3141-26-2, 3,4-Dibromothiophene
RL: RCT (Reactant); RACT (Reactant or reagent)
(carboxylation of)
- IT 96-50-4, 2-Aminothiazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorodeamination of)
- IT 693-16-3, 2-Octanamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with acetyl chloride)
- IT 312-94-7, 2-(Trifluoromethyl)benzoyl chloride 393-52-2, 2-Fluorobenzoyl chloride 393-82-8, 2,5-Bis(trifluoromethyl)benzoyl chloride 874-60-2, 4-Methylbenzoyl chloride 1711-07-5, 3-Fluorobenzoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with amines)
- IT 18063-02-0, 2,6-Difluorobenzoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminomethylpropanol)
- IT 57-14-7, 1,1-Dimethylhydrazine 95-53-4, 2-Methylaniline, reactions 110-76-9, 2-Ethoxyethylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with benzoyl chloride deriv.)
- IT 95-14-7, 1H-Benzotriazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with benzoyl chloride deriv. and benzaldehyde)
- IT 100-52-7, Benzaldehyde, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with benzoyl chloride deriv. and benzotriazole)
- IT 14610-37-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with benzoyl chlorides)
- IT 814-49-3, Diethyl chlorophosphate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with ethylamine)
- IT 123-75-1, Pyrrolidine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with fluorobenzoyl chloride)
- IT 13117-94-7, 2-tert-Butyl-6-methylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with formic acid)
- IT 527-72-0, 2-Thiophenecarboxylic acid 6973-60-0, 1-Methyl-2-pyrrolicarboxylic acid 21739-92-4
RL: PROC (Process)
(conversion of, to acid chloride)
- IT 35730-09-7, 2,5-Difluorobenzoyl chloride
RL: PROC (Process)
(conversion of, to benzamide)
- IT 454-92-2, 3-(Trifluoromethyl)benzoic acid 947-84-2, 2-Phenylbenzoic acid 21739-93-5, 2-Bromo-5-chlorobenzoic acid
RL: PROC (Process)
(conversion of, to benzamide via acid chloride)
- IT 3320-83-0, o-Chlorophenyl isocyanate
RL: PROC (Process)
(conversion of, to carbamate ester)

- IT 88-13-1, Thiophene-3-carboxylic acid
RL: PROC (Process)
(conversion of, to carboxamide via acid chloride)
- IT 55-22-1, 4-Pyridinecarboxylic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion of, to carboxamide via acid chloride)
- IT 1918-79-2, 5-Methyl-2-thiophenecarboxylic acid 24065-33-6,
5-Chloro-2-thiophenecarboxylic acid
RL: PROC (Process)
(conversion of, to silylated carboxamide deriv. via acid chloride)
- IT 78-93-3, Ethyl methyl ketone, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion of, to thiophenecarboxamide)
- IT 90-11-9, 1-Bromonaphthalene 95-46-5, 2-Bromotoluene 573-17-1,
9-Bromophenanthrene 580-13-2, 2-Bromonaphthalene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with benzazaborolone)
- IT 60-34-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with (ethoxymethylene)cyanoacetate)
- IT 62-56-6, Thiourea, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with Et pyruvate)
- IT 108-94-1, Cyclohexanone, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with cyanoacetate and sulfur, in prepn. of fungicides)
- IT 105-56-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with cyclohexanone and sulfur, in prepn. of fungicides)
- IT 94-05-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with methylhydrazine)
- IT 70-23-5, Ethyl bromopyruvate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with thiourea)
- IT 107-09-5, 2-Bromoethylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with bromoethylamine)
- IT 88-67-5, 2-Iodobenzoic acid 59748-90-2, 4-Bromo-2-chlorobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with hexamethyldisilazane)
- IT 630-19-3, Trimethylacetaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(imination of)
- IT 271-58-9, Anthranil
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidative alkylation of)
- IT 150079-80-4P 150079-82-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and acidic ring cleavage of)
- IT 150079-72-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and alkylation of)
- IT 609-67-6P, 2-Iodobenzoyl chloride 5271-67-0P, 2-Thiophenecarboxylic acid chloride 5952-92-1P 16099-04-0P 16372-51-3P 16694-17-0P,
4-Bromo-3-thiophenecarboxylic acid 21900-52-7P 26214-68-6P
41507-35-1P, 3-Thiophenecarbonyl chloride 91489-09-7P 150079-78-0P
150079-86-0P 150108-56-8P 150108-58-0P 150108-59-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and amidation of)
 IT 150108-71-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and amine deprotection of)
 IT 150108-72-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and arom. chloride substitution of)
 IT 65861-69-0P 150079-90-6P 150108-75-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and arom. chlorination of)
 IT 10601-63-5P, N-Isopropylpropionamide 23602-00-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and borane redn. of, to amine)
 IT 4506-71-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and bromination of)
 IT 3034-52-4P, 2-Chlorothiazole
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and carboxylation of)
 IT 5398-36-7P, Ethyl 2-amino-4-thiazolecarboxylate
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and chlorodeamination of)
 IT 150079-39-3P 150079-49-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and condensation of, with amines)
 IT 150079-63-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with benzaldehyde and benzotriazole)
 IT 57440-88-7P 131932-72-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with benzoyl chloride deriv.)
 IT 150079-65-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and condensation of, with trichloroacetyl chloride)
 IT 150108-60-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to (hydroxymethyl)thiophenecarboxamide)
 IT 150108-54-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to acetyl deriv.)
 IT 5198-87-8P, 2-Chloro-4-thiazolecarboxylic acid 78764-55-3P
150079-25-7P 150079-27-9P 150079-38-2P 150079-48-4P
 150079-77-9P 150079-85-9P 150108-55-7P 150108-57-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to acid chloride)
 IT 31562-07-9P **150079-26-8P** 150079-28-0P 150079-50-8P
 150079-51-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to benzamide)
 IT 150079-56-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to benzamide deriv.)
 IT 1077-58-3P, 2-tert-Butylbenzoic acid
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to benzamide deriv. via acid chloride)
 IT 22921-68-2P, 2-Bromo-5-methoxybenzoic acid 150079-84-8P 150079-89-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to benzamide via acid chloride)

IT 100523-84-0P 150108-63-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to carboxamide via acid chloride)

IT 57021-53-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to tetrahydrobenzothiophenecarboxylate)

IT 31562-01-3P 150079-74-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to .beta.-lactam)

IT 150108-78-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and coupling of, with org. bromides)

IT 31037-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and deamination of)

IT 150079-35-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and dehydration of)

IT 59147-01-2P, Trimethylsilyl 2-iodobenzoate 150079-76-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and desilylation of)

IT 150079-36-0P 150079-57-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and ethylation of)

IT 150079-52-0P 150079-53-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and fluorination of)

IT 150079-79-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and formylation of)

IT 55523-45-0P 62924-92-9P 85370-65-6P 97308-13-9P 121424-93-9P
121425-02-3P 121425-03-4P 146516-68-9P 150076-57-6P 150076-58-7P
150076-59-8P 150076-60-1P 150076-61-2P 150076-62-3P 150076-63-4P
150076-64-5P 150076-65-6P 150076-66-7P 150076-67-8P 150076-68-9P
150076-69-0P 150076-70-3P 150076-71-4P 150076-72-5P 150076-73-6P
150076-74-7P 150076-75-8P 150076-76-9P 150076-77-0P 150076-78-1P
150076-79-2P 150076-80-5P 150076-81-6P 150076-82-7P 150076-83-8P
150076-84-9P 150076-85-0P 150076-86-1P 150076-87-2P 150076-88-3P
150076-89-4P 150076-90-7P 150076-91-8P 150076-92-9P 150076-93-0P
150076-94-1P 150076-95-2P 150076-96-3P 150076-97-4P 150076-98-5P
150076-99-6P 150077-00-2P 150077-01-3P 150077-02-4P 150077-03-5P
150077-04-6P 150077-05-7P 150077-06-8P 150077-07-9P 150077-08-0P
150077-09-1P 150077-10-4P 150077-11-5P 150077-12-6P 150077-13-7P
150077-14-8P 150077-15-9P 150077-16-0P 150077-17-1P 150077-18-2P
150077-19-3P 150077-20-6P 150077-21-7P 150077-22-8P 150077-23-9P
150077-24-0P 150077-25-1P 150077-26-2P 150077-27-3P 150077-28-4P
150077-29-5P 150077-30-8P 150077-31-9P 150077-32-0P 150077-33-1P
150077-34-2P 150077-35-3P 150077-36-4P 150077-37-5P 150077-38-6P
150077-39-7P 150077-40-0P 150077-41-1P 150077-42-2P 150077-43-3P
150077-44-4P 150077-45-5P 150077-46-6P 150077-47-7P 150077-48-8P
150077-49-9P 150077-50-2P 150077-51-3P 150077-52-4P 150077-53-5P
150077-54-6P 150077-55-7P 150077-56-8P 150077-57-9P 150077-58-0P
150077-59-1P 150077-60-4P 150077-61-5P 150077-62-6P 150077-63-7P
150077-64-8P 150077-65-9P 150077-66-0P 150077-67-1P 150077-68-2P
150077-69-3P 150077-70-6P 150077-71-7P 150077-72-8P 150077-73-9P
150077-74-0P 150077-75-1P 150077-76-2P 150077-77-3P 150077-78-4P

| | | | | |
|--------------|--------------|--------------|--------------|--------------|
| 150077-79-5P | 150077-80-8P | 150077-81-9P | 150077-82-0P | 150077-83-1P |
| 150077-84-2P | 150077-85-3P | 150077-86-4P | 150077-87-5P | 150077-88-6P |
| 150077-89-7P | 150077-90-0P | 150077-91-1P | 150077-92-2P | 150077-93-3P |
| 150077-94-4P | 150077-95-5P | 150077-96-6P | 150077-97-7P | 150077-98-8P |
| 150077-99-9P | 150078-00-5P | 150078-01-6P | 150078-02-7P | 150078-03-8P |
| 150078-04-9P | 150078-05-0P | 150078-06-1P | 150078-07-2P | 150078-08-3P |
| 150078-09-4P | 150078-10-7P | 150078-11-8P | 150078-12-9P | 150078-13-0P |
| 150078-14-1P | 150078-15-2P | 150078-16-3P | 150078-17-4P | 150078-18-5P |
| 150078-19-6P | 150078-20-9P | 150078-21-0P | 150078-22-1P | 150078-23-2P |
| 150078-24-3P | 150078-25-4P | 150078-26-5P | 150078-27-6P | 150078-28-7P |
| 150078-29-8P | 150078-30-1P | 150078-31-2P | 150078-32-3P | 150078-33-4P |
| 150078-34-5P | 150078-35-6P | 150078-36-7P | 150078-37-8P | 150078-38-9P |
| 150078-39-0P | 150078-40-3P | 150078-41-4P | 150078-42-5P | 150078-43-6P |
| 150078-44-7P | 150078-45-8P | 150078-46-9P | 150078-47-0P | 150078-48-1P |
| 150078-49-2P | 150078-50-5P | 150078-51-6P | 150078-52-7P | 150078-53-8P |
| 150078-54-9P | 150078-55-0P | 150078-56-1P | 150078-57-2P | 150078-58-3P |
| 150078-59-4P | 150078-60-7P | 150078-62-9P | 150078-63-0P | 150078-64-1P |
| 150078-65-2P | 150078-66-3P | 150078-67-4P | 150078-68-5P | 150078-69-6P |
| 150078-70-9P | 150078-71-0P | 150078-72-1P | 150078-73-2P | 150078-74-3P |
| 150078-75-4P | 150078-76-5P | 150078-77-6P | 150078-78-7P | 150078-79-8P |
| 150078-80-1P | 150078-81-2P | 150078-82-3P | 150078-83-4P | 150078-84-5P |
| 150078-85-6P | | | | |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and fungicidal activity of, in control of take-all disease of plants)

| | | | | | |
|----|--------------|--------------|--------------|--------------|--------------|
| IT | 150078-87-8P | 150078-88-9P | 150078-89-0P | 150078-90-3P | 150078-91-4P |
| | 150078-92-5P | 150078-93-6P | 150078-94-7P | 150078-95-8P | 150078-96-9P |
| | 150078-98-1P | 150078-99-2P | 150079-00-8P | 150079-01-9P | 150079-02-0P |
| | 150079-03-1P | 150079-04-2P | 150079-05-3P | 150079-06-4P | 150079-07-5P |
| | 150079-08-6P | 150079-09-7P | 150079-10-0P | 150079-11-1P | 150079-12-2P |
| | 150079-13-3P | 150079-14-4P | 150079-15-5P | 150079-16-6P | 150079-17-7P |
| | 150079-18-8P | 150079-19-9P | 150079-20-2P | 150079-21-3P | 150079-22-4P |
| | 150079-23-5P | 150079-24-6P | 150108-45-5P | 150108-46-6P | |
| | 150108-47-7P | 150108-48-8P | 150108-49-9P | 150108-50-2P | 150144-98-2P |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and fungicidal activity of, in control of take-all disease of plants)

IT 150079-31-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and intramol. cyclocondensation of)

IT 150079-34-8P 150079-58-6P 150079-69-9P 150079-70-2P 150108-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and methylation of)

IT 150079-45-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and oxazoline ring cleavage of, with anhydride)

IT 150079-81-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and oxidn. of)

IT 150108-61-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and oxidn. of, to formyl deriv.)

IT 150108-62-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
 (prepn. and oxidn. of, with periodate)

IT 150079-75-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with amine)

IT 1946-09-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with benzoyl chloride deriv.)

IT 150079-60-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with cyanoborohydride)

IT 10345-79-6P 66896-65-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with electrophile)

IT 150079-64-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with isopropylamine)

IT 150108-76-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with isopropylhydroxylamine)

IT 150079-62-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with triethylamine, benzenecarboximidothioate
 from)

IT 87306-63-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with trifluoromethanesulfonic anhydride)

IT 66464-26-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reactions of)

IT 117054-83-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and redn. of, to amine)

IT 14559-12-7P 19156-54-8P 41731-52-6P, Ethyl 2-chloro-4-
 thiazolecarboxylate 85290-80-8P 139287-38-0P 150079-47-3P
 150108-66-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and sapon. of)

IT 5980-28-9P 10366-86-6P 14657-86-4P, N,N-Dipropylbenzamide
 15952-65-5P 41116-48-7P 66896-66-0P 69919-07-9P 97010-05-4P
 98547-26-3P 124725-22-0P 150079-37-1P 150079-55-3P 150079-61-1P
 150079-66-6P 150079-67-7P 150079-68-8P 150079-83-7P 150079-87-1P
 150079-91-7P 150079-92-8P 150108-51-3P 150108-53-5P 150108-64-8P
 150108-65-9P 150108-68-2P 150108-70-6P 150108-73-9P 150108-74-0P
 150108-77-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and silylation of)

IT 150079-71-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and substitution of, with chloride)

IT 52559-62-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and thermal rearrangement of, benzonitrile deriv. from)

IT 134-62-3P 2728-05-4P 35426-69-8P 57547-96-3P 131401-55-3P
150079-33-7P 150079-40-6P 150079-41-7P 150079-42-8P 150079-43-9P
150079-44-0P 150079-54-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and trimethylsilylation of)

IT 91202-03-8P 139287-30-2P 150079-46-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and N-methylation of)

IT 41882-26-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tert-butoxylation of)

IT 150108-67-1P 150108-69-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 52135-87-2P 142551-31-3P 150079-29-1P 150079-30-4P 150079-32-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate to fungicide compd.)

IT 10271-85-9P, 5-Isothiazolecarboxylic acid 101012-12-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., amidation, and subsequent silylation of)

IT 150079-88-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., deesterification, and arom. silylation of)

IT 121424-94-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., methylation, and fungicidal activity of, in control of take-all disease of plants)

IT 150078-61-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., reactions, and fungicidal activity of, in control of take-all disease of plants)

IT 150078-97-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., redn., and fungicidal activity of, in control of take-all disease of plants)

IT 150078-86-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., thiolation, and fungicidal activity of, in control of take-all disease of plants)

IT 109-97-7, Pyrrole 288-13-1, Pyrazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et isocyanate)

IT 387-45-1, 2-Chloro-6-fluorobenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with azide, chloroanthranil from)

IT 2373-51-5, Chloromethyl methyl sulfide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzamide)

IT 66464-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with electrophiles)

IT 609-65-4, 2-Chlorobenzoyl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methyleneimine)

IT 109-90-0, Ethyl isocyanate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with pyrrole)

IT 768-33-2, Chlorodimethylphenylsilane 1719-58-0, Dimethyl(vinyl)silyl
 chloride 3634-56-8, Chloroisopropyldimethylsilane 4028-23-3,
 Allylchlorodimethylsilane 18162-48-6, tert-Butylchlorodimethylsilane
 18162-84-0, Chlorodimethyloctylsilane 71864-47-6,
 Chlorocyclohexyldimethylsilane 117046-42-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (silylation by, of benzamide)

IT 17306-05-7, Chloromethylphenylvinylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (silylation by, of benzamide deriv.)

IT 1719-57-9, (Chloromethyl)dimethylsilyl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (silylation by, of benzamides)

IT 75-66-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (thiolation by, of (difluorophenyl)dimethyloxazoline)

IT 40167-20-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (thiolation by, of benzamide deriv.)

IT 50-45-3, 2,3-Dichlorobenzoic acid 88-65-3, 2-Bromobenzoic acid
 118-91-2, 2-Chlorobenzoic acid 488-93-7, 3-Furoic acid 614-17-5,
 N-Ethylbenzamide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (trimethylsilylation of)

L199 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1993:516522 HCAPLUS

DN 119:116522

TI Preparation of **alpha-halo enamines** from
 carboxamides and phosphorus oxychloride or -bromide

IN Ghosez, Leon; Koch, Isabelle George

PA Ciba-Geigy A.-G., Switz.

SO Patentschrift (Switz.), 7 pp.

CODEN: SWXXAS

DT Patent

LA German

IC ICM C07C209-74

ICS C07D207-00; C07D211-00; C07D265-28

CC 21-2 (General Organic Chemistry)

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|----------|
| PI | CH 681623 | A | 19930430 | CH 1990-3501 | 19901105 |
| OS | CASREACT 119:116522; MARPAT 119:116522 | | | | |
| AB | A process for the prepn. of .alpha.-chloro or .alpha.-bromo enamines , i.e., R1R2C: CXNR3R4 [R1, R2, R3, R4 = various (un)substituted hydrocarbonyl groups; or R1R2 = (un)substituted alkylene; or R3R4 = (CH2)4, (CH2)5, CH2CH2OCH2CH2, etc.; R3, R4 may connect to an addnl. enamine moiety; X = Cl, Br], comprises treatment of carboxamides having an .alpha.-hydrogen to the carbonyl group, i.e., R1R2CHC(O)NR3R4, with POCl3 or POBr3, resp., first in the presence of a catalytic amt. of an N,N-disubstituted amide (formamide or .alpha.-methylenic carboxamide), or an N-substituted .alpha.-methylenic lactam, and then in the presence of a tertiary amine ,. E.g., 1-(dimethylamino)-1- chloro -2-methylprop-1-ene was prepd. from POCl3 and N,N,2-trimethylpropionamide in CH2Cl2 in the presence of a small amt. of DMF, in the subsequent presence of Et3N, in 90% yield. | | | | |

- ST **enamine alpha halo**; carboxamide conversion
chloro enamine phosphorus oxychloride; amide conversion
bromo enamine phosphorus oxybromide
- IT Amides, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactions of, with phosphorus oxyhalides, **.alpha.-halo enamines** from)
- IT **Enamines**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (**halo**, prepn. of, from carboxamides and phosphorus oxyhalides)
- IT 26189-59-3P 58933-80-5P 58933-81-6P
 60180-60-1P 65785-45-7P 72184-21-5P
 72184-22-6P 73630-93-0P 87443-04-7P
 116437-56-0P 149554-68-7P 149554-69-8P
 149554-70-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- IT 957-51-7 6282-98-0 17566-51-7 18071-39-1 18940-58-4 21678-37-5
 33931-47-4 55577-65-6 149554-71-2 149554-72-3 149554-73-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with phosphorus oxyhalide, **.alpha.-halo enamine** from)
- L199 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2002 ACS
 AN 1990:98997 HCAPLUS
 DN 112:98997
 TI Preparation of glycosyl halides under neutral conditions
 AU Ernst, Beat; Winkler, Tammo
 CS Cent. Res. Lab., Ciba-Geigy Ltd., Basel, CH 4002, Switz.
 SO Tetrahedron Lett. (1989), 30(23), 3081-4
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 CC 33-2 (Carbohydrates)
 OS CASREACT 112:98997
 AB The anomeric hydroxyl group of various furanose and pyranose hemiacetals can be replaced by a **fluorine, chlorine, bromine** or **iodine** atom under neutral conditions using **haloenamines**. Thus, 2,3,4,6-tetra-O-benzyl-D-glucopyranose was treated with Me2C:C(NMe2)Cl in CHCl3 for 6 h to give 92% 2,3,4,6-tetra-O-benzyl-**.alpha.-D-glucopyranosyl chloride**
- ST glycosyl halide; **halogenation** furanose pyranose
haloenamine; **enamine halo halogenation**
 pyranose
- IT **Halogenation**
 (of glycopyranose and glycofuranoses with **haloenamines**)
- IT Carbohydrates and Sugars, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (glycosyl halides, prepn. of, under neutral conditions)
- IT 26189-59-3 65560-29-4 65560-41-0
 65785-54-8 73630-93-0
 RL: RCT (Reactant)
 (**halogenation** by, of glycopyranose or glycofuranoses)
- IT 38768-81-9 40036-82-6 40437-08-9 58645-20-8 77668-10-1
 125181-26-2
 RL: RCT (Reactant)
 (**halogenation** of, with **haloenamines**)
- IT 440-03-9P 572-09-8P 2823-44-1P 2823-46-3P 3934-29-0P 4196-35-4P
 4451-35-8P 6919-97-7P 13035-49-9P 13242-53-0P 14227-51-1P
 14227-66-8P 14257-40-0P 17087-84-2P 20720-33-6P 21085-72-3P
 25320-59-6P 38838-12-9P 53008-62-1P 57573-38-3P 78153-79-4P

89025-46-7P 94898-41-6P 96089-62-2P 108800-87-9P 116523-80-9P
125181-24-0P 125181-25-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L199 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1985:131224 HCAPLUS

DN 102:131224

TI A development of highly selective synthetic reactions via iminium salts

AU Fujisawa, Tamotsu; Sato, Toshio

CS Fac. Eng., Mie Univ., Tsu, 514, Japan

SO Kenkyu Hokoku - Asahi Garasu Kogyo Gijutsu Shoreikai (1984), 44, 83-94

CODEN: AGKGAA; ISSN: 0365-2599

DT Journal; General Review

LA Japanese

CC 21-0 (General Organic Chemistry)

AB A review with 14 refs. on the use of **haloiminium** salts or .

alpha.-haloenamines as condensation reagents for chemoselective reactions of activated carboxylic acids, nitroalkanes, and alcs.

ST review iminium salt reaction

IT Iminium compounds

RL: RCT (Reactant)

(synthetic reactions via)

L199 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1983:179443 HCAPLUS

DN 98:179443

TI .beta.-Lithiated **enamines**. I. Preparations and alkylation reactions

AU Duhamel, Lucette; Poirier, Jean Marie

CS Lab. Chim. Org., Fac. Sci. Tech. Rouen, Mont-Saint-Aignan, F-76130, Fr.

SO Bull. Soc. Chim. Fr. (1982), (9-10, Pt. 2), 297-303

CODEN: BSCFAS; ISSN: 0037-8968

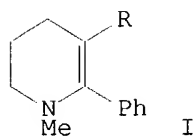
DT Journal

LA French

CC 29-2 (Organometallic and Organometalloidal Compounds)

OS CASREACT 98:179443

GI



AB Treating .beta.-**bromo**enamine with Me₃CLi or BuLi in THF at -70.degree. gave .beta.-**lithio**enamine via **halogen**-metal exchange. Thus, treating MeCBr:CHNET₂ or II (R = Br) with Me₃CLi gave MeCLi:CHNET₂ or I (R = Li), resp. Use of metallic Li instead of organolithium reagents resulted in the formation of small amts. of byproducts. Treating Me₂NCPPh:CHCl with RLi (R1 = Bu, Me₃C) gave Me₂NCPPh:CR1Cl, which reacted with electrophiles to form the substituted **enamines**. The .beta.-**lithio**enamines studied are stable compds. even up to 20.degree. in most cases. Their reactions to form .beta.-substituted **enamines**, or by hydrolysis, .**alpha**.-substituted carbonyl compds., were studied.

ST **enamine bromo** lithiation; **lithio**enamine reaction

IT Stereochemistry

- (of reaction of **.beta.-lithioenamine** with alkyl halides)
- IT Lithiation
(of **.beta.-haloenamines**)
- IT Alkylation
(of **.beta.-lithioenamines**)
- IT Carbonyl compounds, preparation
RL: PREP (Preparation)
(**.alpha.-substituted**, by hydrolysis of **enamines**)
- IT **Enamines**
RL: RCT (Reactant)
(**.beta.-halo-**, lithiation of)
- IT 76906-47-3 85429-47-6
RL: PRP (Properties)
(NMR spectrum of)
- IT 74-88-4, reactions 75-03-6 542-69-8
RL: RCT (Reactant)
(alkylation by, of **.beta.-lithioenamine**)
- IT 14548-16-4
RL: RCT (Reactant)
(**bromination** and reaction with butyllithium)
- IT 7439-93-2, reactions
RL: RCT (Reactant)
(lithiation by, of **.beta.-bromoenamine**)
- IT 594-19-4 109-72-8P, preparation
RL: RCT (Reactant)
(lithiation by, of **.beta.-haloenamines**)
- IT 21411-45-0 61170-34-1 61214-42-4 65174-17-6 71129-92-5
76906-37-1 76906-48-4 85429-28-3 85429-29-4 85429-30-7
RL: RCT (Reactant)
(lithiation of, by alkyllithium reagents)
- IT 85429-48-7P 85437-49-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with electrophiles)
- IT 85429-35-2P 85429-36-3P 85429-37-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reactions of)
- IT 93-55-0P 564-04-5P 942-92-7P 1590-08-5P 17180-39-1P 22502-84-7P
27610-88-4P 33119-75-4P 57847-43-5P 71130-00-2P 84395-66-4P
85429-31-8P 85429-32-9P 85429-33-0P 85429-34-1P 85429-38-5P
85429-39-6P 85429-40-9P 85429-41-0P 85429-42-1P 85429-43-2P
85429-44-3P 85429-45-4P 85429-46-5P 85429-49-8P 85429-50-1P
85429-51-2P 85429-52-3P 85429-53-4P 85429-54-5P 85429-55-6P
85429-56-7P 85429-57-8P 85429-58-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 30263-73-1
RL: RCT (Reactant)
(prepn. of **bromoenamine** from)
- IT 7784-34-1
RL: RCT (Reactant)
(reaction of, with **bromodimethylbutanal**, **bromoenamine** from)
- IT 6596-96-9
RL: RCT (Reactant)
(reaction of, with **chloroacetophenone**)
- IT 532-27-4
RL: RCT (Reactant)
(reaction of, with tris(dimethylamino)arsine)

L199 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1982:492398 HCAPLUS

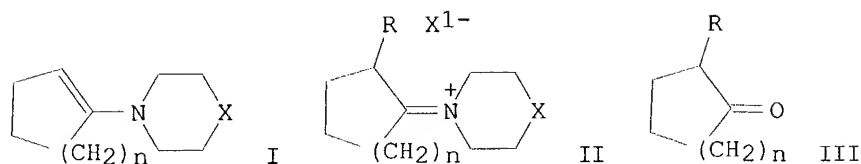
DN 97:92398

TI Stereospecific **halogenation** of ethyl methyl phosphorothioates

- AU Hall, C. Richard; Williams, Nancy E.
 CS Chem. Def. Establ., Salisbury, SP4 0JQ, UK
 SO Tetrahedron Lett. (1982), 23(9), 999-1002
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 23
 OS CASREACT 97:92398
 AB The stereospecific **halogenation** of (R)-(+)-HSP(O)(OMe)OEt (I) with tetramethyl-**.alpha.-haloenamines** is reported. Treating I with Me₂C:CRNMe₂ (R = F, Cl, Br) gave (S)-(+)-RP(O)(OEt)OMe (II; same R) stereospecifically, together with Me₂CHCSNMe₂. The reaction mechanism is discussed. The stereochem. of the substitution reactions of the phosphoryl halides II was studied. E.g., substitution reaction of II (R = Cl) with NaOPh gave enantiomerically pure (R)-(+)-PhOP(O)(OEt)OMe, whereas that of II (R = Cl) with NaON:CMe₂ gave (R)-(-)-Me₂C:NOP(O)(OMe)OEt, which underwent substitution reaction with NaOCHMe₂ to give (S)-(+)-Me₂CHOP(O)(OMe)OEt.
- ST **halogenation** phosphorothioate **haloenamine** stereospecificity; substitution phosphoryl halide stereochem; **enamine halo halogenation** phosphorothioate
- IT **Halogenation**
 (of Et Me phosphorothioate with **tetramethylhaloenamines**, stereospecific)
- IT Stereochemistry
 (of **halogenation** of Et Me phosphorothioates with **tetramethylhaloenamines**)
- IT Substitution reaction, nucleophilic
 (of phosphoryl halides with phenoxide ion and acetone oxime, stereochem. of)
- IT **Enamines**
 RL: RCT (Reactant)
 (**halo, halogenation** of Et Me phosphorothioate with, stereospecific)
- IT 26189-59-3 65560-29-4 73630-93-0
 RL: RCT (Reactant)
 (**halogenation** of Et Me phosphorothioate with, stereospecific)
- IT 71348-05-5
 RL: RCT (Reactant)
 (**halogenation** of, with tetramethyl-**.alpha.-haloenamines**, stereospecific)
- IT 82765-14-8P 82765-15-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and methylation of)
- IT 82765-13-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and substitution reaction of, with isopropoxide)
- IT 71348-14-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and substitution reactions of, stereospecificity of)
- IT 52912-63-7P 57557-25-2P 71348-16-8P 82765-12-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- IT 64415-67-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, by substitution reaction of phosphoryl **chloride** with phenoxide, stereospecificity of)
- IT 57557-32-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, by substitution reactions of phosphoryl **chloride**, stereospecificity of)
- IT 71348-06-6

- RL: RCT (Reactant)
(substitution reactions of, stereospecific)
- IT 139-02-6 683-60-3 824-78-2 75392-06-2
RL: RCT (Reactant)
(substitution reactions of, with phosphoryl chlorides,
stereospecific)
- L199 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1980:567532 HCAPLUS
DN 93:167532
TI **.alpha.-Chloro enamines, reactive
intermediates for synthesis: 1-chloro
-N,N,2-trimethylpropenylamine**
AU Haveaux, B.; Dekoker, A.; Rens, M.; Sidani, A. R.; Toye, J.; Ghosez, L.
CS Lab. Chim. Org. Synth., Univ. Louvain, Louvain-La-Neuve, B-1348, Belg.
SO Org. Synth. (1980), 59, 26-34
CODEN: ORSYAT; ISSN: 0078-6209
DT Journal
LA English
CC 23-4 (Aliphatic Compounds)
AB RR1C:CC1NR2R3 [R = Me, Ph, H, R1 = H, R2 = Me, R3 = Ph; R = Me3C, Me, Ph,
R1 = H, Me, R2 = R3 = Me; R = R1 = Me, R2R3 = (CH2)5; RR1 = (CH2)5, R2R3 =
Et; R = Me, R1 = Cl, R2R3 = (CH2)4; R = R3 = Me, R1R2 = (CH2)4] were
prepd. in 40-85% yields by treating RR1CHCONR2R3 with COCl2 to give
RR1CHCCl:N+R2R3.Cl-, which was refluxed in CH2Cl2 in the presence of Et3N
for 1 h.
ST alkylamide **chlorination** phosgene safety; **chloroenamine**
; **enamine chloro**; **chloroalkylidenium**
chloride prepn dehydrochlorination
IT Amides, reactions
RL: RCT (Reactant)
(**chlorination** of, by phosgene, **.alpha.-**
chloroenamine from)
IT Safety
(in handling of phosgene)
IT **Enamines**
(**.alpha.-chloro**, prepn. of, from amides)
IT 75-44-5
RL: RCT (Reactant)
(**chlorination** of alkylamide by)
IT 563-83-7 579-10-2 5461-52-9 5827-78-1 17201-04-6 26153-90-2
40669-47-4 41836-85-5 55577-65-6 55917-05-0 75115-52-5
RL: RCT (Reactant)
(**chlorination** of, by phosgene)
IT 52851-35-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation)
(prepn. and dehydrochlorination of)
IT 23150-97-2P 26189-59-3P 58933-81-6P
65785-52-6P 65785-53-7P 74044-20-5P
75115-53-6P 75115-54-7P 75115-55-8P
75115-56-9P 75115-57-0P 75115-58-1P
75115-59-2P 75115-60-5P 75125-74-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- L199 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1979:438957 HCAPLUS
DN 91:38957
TI **Halogenation of enamines - synthesis of .beta.-**
halo iminium halides
AU Seufert, Walter; Effenberger, Franz
CS Inst. Org. Chem., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.

SO Chem. Ber. (1979), 112(5), 1670-6
 CODEN: CHBEAM; ISSN: 0009-2940
 DT Journal
 LA German
 CC 24-1 (Alicyclic Compounds)
 GI



AB The **enamines** I (X = bond, CH₂, O; n = 1, 2, 3) reacted with Br, Cl, or **iodine** to give the iminium halides II (X₁ = R = Cl, Br, I), which were hydrolyzed to the **.alpha.-halo** ketones III.

ST **halogenation** aminocycloalkene; iminium halide
halocycloalkane; cycloalkanone **halo**

IT **Halogenation**

(of aminocycloalkanones, iminium halide from)

IT 670-80-4 936-52-7 1125-99-1 1614-92-2 2981-10-4 7148-07-4
 7182-08-3 14092-11-6 19353-04-9

RL: RCT (Reactant)

(**halogenation** of, iminium halide from)

IT 70742-75-5P 70742-76-6P 70742-77-7P 70742-78-8P 70742-79-9P
 70742-80-2P 70742-81-3P 70742-82-4P 70742-83-5P 70742-84-6P
 70742-85-7P 70742-86-8P 70742-87-9P 70742-88-0P 70742-89-1P
 70742-90-4P 70742-91-5P 70742-92-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and hydrolysis of)

IT 694-28-0P 766-65-4P 766-66-5P 822-85-5P 822-87-7P 21943-50-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, by hydrolysis of **haloiminium** halide)

L199 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1978:104640 HCAPLUS

DN 88:104640

TI Reactivity and synthetic potential of **.alpha.-fluoro-**
and .alpha.-iodoenamines

AU Colens, Alain; Ghosez, Leon

CS Lab. Chim. Synth., Univ. Louvain, Louvain, Belg.

SO Nouv. J. Chim. (1977), 1(5), 371-2

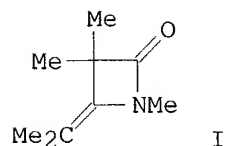
CODEN: NJCHD4

DT Journal

LA English

CC 23-18 (Aliphatic Compounds)

GI

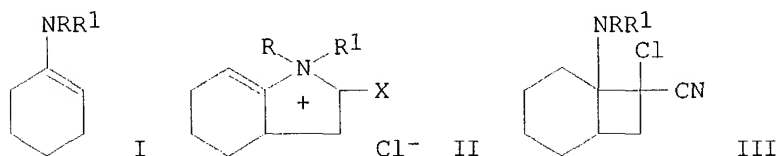


- AB The nucleophilic character of **.alpha.-fluoroenamines** and the electrophilic character of **.alpha.-iodoenamines** was shown. E.g., Me2C:CFNMe2 reacted with Me2C:CINMe2 in HCCl3 at 20.degree. to give, after hydrolysis, the **.beta.-lactam I**.
- ST nucleophilicity **fluoroenamine**; electrophilicity **iodoenamine**; **enamine halo** reaction; **lactam beta isopropylidene**
- IT Electrophilicity
Nucleophilicity
(of **.alpha.-haloenamines**)
- IT Amines, reactions
(**.alpha.-haloenamines**, reactions of, electro- or nucleophilic character in)
- IT **65560-33-0**
RL: RCT (Reactant)
(condensation of, with malononitrile)
- IT 109-77-3
RL: RCT (Reactant)
(condensation of, with **.alpha.-fluoroenamine**)
- IT **65560-30-7**
RL: RCT (Reactant)
(hydrofluorination of)
- IT 65799-99-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)
- IT 50483-91-5P 55019-20-0P 65560-31-8P 65560-32-9P 65560-34-1P
65560-35-2P 65560-36-3P **65560-38-5P** 65560-39-6P
65560-40-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 75-44-5 79-37-8 421-20-5
RL: RCT (Reactant)
(reaction of, with **.alpha.-fluoroenamine**)
- IT **65560-29-4 65560-41-0**
RL: RCT (Reactant)
(reactions of)
- L199 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2002 ACS
- AN **1978:104595** HCAPLUS
- DN **88:104595**
- TI **Synthesis of .alpha.-fluoro- and .alpha.-iodoenamines**
- AU Colens, Alain; Demuylder, Michel; Techy, Brigitte; Ghosez, Leon
- CS Lab. Chim. Org. Synth., Univ. Louvain, Louvain, Belg.
- SO Nouv. J. Chim. (1977), 1(5), 369-70
CODEN: NJCHD4
- DT Journal
- LA English
- CC 23-3 (Aliphatic Compounds)
- AB RCR1:C(NR2R3)Cl [R and R1 (same or different) are Me, Ph, Et, Cl; R2 and R3 (same or different) are Me, CHMe2, Ph; and NR2R3 = morpholino] were treated with KF and KI to give the resp. RCR1:C(NR2R3)F and RCR1:C(NR2R3)I.
- ST **chlorovinylamine halogen** exchange; **enamine chloro halogen** exchange; **fluoro enamine**; **iodo enamine**
- IT Exchange reaction
(**halogen**, of N-(1-chlorovinyl)dialkylamines with potassium **fluoride** and potassium **iodide**)
- IT 4231-35-0
RL: RCT (Reactant)
(addn. reaction of, with potassium **fluoride**)

- IT 58933-80-5 65785-48-0 65785-49-1
65785-50-4 65785-51-5 65785-52-6
65785-53-7
RL: RCT (Reactant)
(halogen exchange reaction of, with potassium fluoride)
- IT 26189-59-3 65785-45-7 65785-46-8
65785-47-9
RL: RCT (Reactant)
(halogen exchange reaction of, with potassium fluoride and potassium iodide)
- IT 65560-29-4P 65560-33-0P 65560-41-0P
65785-54-8P 65785-55-9P 65785-56-0P
65785-57-1P 65785-58-2P 65785-59-3P
65785-60-6P 65785-61-7P 65785-62-8P
65785-63-9P 65785-64-0P 65785-65-1P
65785-66-2P 65785-67-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- L199 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1978:22789 HCAPLUS
DN 88:22789
TI Halogenation of enamines. I. Synthesis of haloketones from enamines. .alpha.-Halogenated pinacolones
AU Carlson, Rolf; Rappe, Christoffer
CS Dep. Org. Chem., Univ. Umea, Umea, Swed.
SO Acta Chem. Scand., Ser. B (1977), B31(6), 485-90
CODEN: ACBOCV
DT Journal
LA English
CC 28-14 (Heterocyclic Compounds (More Than One Hetero Atom))
AB The reactions of 2-morpholino-3,3-dimethyl-1-butene (I) with Cl and Br were studied under varying conditions for possible transformations to mono- and dihalo ketones. 1-Chloro-3,3-dimethyl-2-butane was prepd. in 42% yield by this method. The usefulness and limitations of the reaction of I with halogens for obtaining halo ketones were briefly discussed.
- ST enamine halogenation; morpholinodimethylbutene halogenation
- IT Halogenation
(of morpholinodimethylbutene)
- IT 5469-26-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and chlorination by sulfuryl chloride)
- IT 22502-84-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and halogenation of)
- IT 13547-70-1P 22591-21-5P 30263-65-1P 36965-30-7P 64984-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 75-97-8
RL: RCT (Reactant)
(reaction of, with morpholine and titanium chloride)
- IT 110-91-8, reactions
RL: RCT (Reactant)
(reaction of, with pinacolone and titanium chloride)
- L199 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1977:139743 HCAPLUS
DN 86:139743
TI Enamine chemistry. XV. The reaction of enamines with

.alpha.-halo electrophilic olefins

AU Madsen, J. O.; Lawesson, S. O.
 CS Chem. Inst., Univ. Aarhus, Aarhus, Den.
 SO Bull. Soc. Chim. Belg. (1976), 85(10), 805-17
 CODEN: BSCBAG
 DT Journal
 LA English
 CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
 GI



AB Reaction of **enamines** I (RR1 = (CH2)2O(CH2)2, (CH2)5, (CH2)4, (CH2)6, (CH2)4CHMe; R = R1 = Me, Et, Bu, Me2CHCH2; R = Me, R1 = Me2CHCH2, cyclohexyl; R = Et, R1 = Bu) with H2C:XCX1 (X = CN, CO2Me) in polar solvents gave 25-80% indoliums II. In ether at low temp. III were obtained. The pyrrolidine and hexahydroazepine **enamines** were the most reactive and the morpholine **enamines** were the least reactive. II were stable toward bases. Heating III in MeCN gave II.

ST **enamine** cyclocondensation electrophilic olefin; indolium salt;
 cyclohexanone **enamine** reaction **chloroacrylate**

IT **Enamines**
 RL: RCT (Reactant)
 (cycloaddn. reaction of, with **.alpha.-halo**
 electrophilic olefins)

IT Alkenes, reactions
 (.alpha.-halo, reaction of, with **enamines**
)

IT 54749-68-7P 62372-36-5P 62372-44-5P 62372-49-0P 62372-50-3P
 62372-51-4P 62372-52-5P 62372-53-6P 62372-54-7P 62372-55-8P
 62372-56-9P 62372-57-0P 62372-58-1P 62372-74-1P 62372-75-2P
 RL: PREP (Preparation)
 (from cyclohexanone **enamine** reaction with electrophilic
 halogenated olefins)

IT 19406-08-7P 62372-69-4P 62372-70-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and conversion of, to indolium salts)

IT 61581-04-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reaction of with acrylonitrile)

IT 49651-43-6P 53516-50-0P 53516-56-6P 62372-47-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reaction of, with **chloroacrylonitrile**)

IT 20215-83-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and redn. of)

IT 51265-33-9P 54749-67-6P 62372-38-7P 62372-40-1P 62372-43-4P
 62372-60-5P 62372-62-7P 62372-64-9P 62372-65-0P 62372-66-1P
 62372-68-3P 62372-71-8P 62372-72-9P 62372-73-0P 62372-76-3P
 62573-47-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 10468-24-3 10468-25-4 13815-46-8 23430-63-9 62372-48-9
 RL: RCT (Reactant)
 (reaction of, with **chloroacrylonitrile**)

- IT 670-80-4
RL: RCT (Reactant)
(reaction of, with **chloroacrylonitrile** and methyl **chloroacrylate**)
- IT 80-63-7 920-37-6
RL: RCT (Reactant)
(reaction of, with cyclohexanone **enamines**)
- IT 1125-99-1 2981-10-4
RL: RCT (Reactant)
(reaction of, with methyl **chloroacrylate**)
- L199 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1977:105179 HCAPLUS
DN 86:105179
TI **.alpha.-Haloenamines** and keteniminium salts
AU Ghosez, L.; Marchand-Brynaert, J.
CS Lab. Chim. Org. Synth., Univ. Louvain, Louvain-la-Neuve, Belg.
SO Adv. Org. Chem. (1976), 9, Pt. 1(Iminium Salts Org. Chem.), 421-532
CODEN: AOMRA7
DT Journal; General Review
LA English
CC 22-0 (Physical Organic Chemistry)
AB A review with 127 refs.
ST review **haloenamine** keteniminium salt; **enamine**
halo review
IT Ketanimines
RL: RCT (Reactant)
(ions, reactions of)
- IT **Enamines**
(**.alpha.-halo**, prepn., reactions, and properties of)
- L199 ANSWER 23 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1976:16445 HCAPLUS
DN 84:16445
TI Action of nucleophilic reagents on **.beta.-haloenamines**
AU Duhamel, Lucette; Poirier, Jean M.
CS Lab. Chim. Org., Fac. Sci. Tech. Rouen, Mont-Saint-Aignan, Fr.
SO Bull. Soc. Chim. Fr. (1975), (1-2, Pt. 2), 329-32
CODEN: BSCFAS
DT Journal
LA French
CC 22-3 (Physical Organic Chemistry)
AB RCX:CHNR12 (I, R = R1 = Et, X = Cl) (II) and MeOH-Et3N gave 60%
RCH(NR12)CH(OMe)2 (III, R = R1 = Et). II and EtSH contg. Et3N gave 50%
RC(SET):CHNR12 (R = R1 = Et). I (R = Me3C, NR12 = morpholino, X = Cl)
with piperidine gave 95% RC(NR12):CHNR22 (IV, R12N = piperidino) and 5% IV
(R12N = morpholino). Treatment of I (R = Me2C, R1 = Me, X = Cl) with
Me3CNH2 gave 55% Me3CCHClCH:NCMe3. III were also prepd. from the
corresponding **.alpha.-halo** iminium salts, which were
intermediates in these reactions, and the alcs. The mechanism of these
reactions was discussed.
ST addn nucleophile **haloenamine**; **enaminehalo** addn
nucleophile
IT Amines, reactions
RL: RCT (Reactant)
(addn., with **.beta.-haloenamines**)
IT Addition reaction
(of **.beta.-haloenamines**, with nucleophiles, mechanism of)
- IT 75-64-9 108-91-8
RL: RCT (Reactant)
(addn. reaction of, with **.beta.-haloenamines**)
- IT 27971-16-0 27971-18-2 27971-19-3 27971-20-6 27971-22-8

27971-24-0 27974-33-0 35593-04-5 35593-06-7 35593-07-8
 35593-09-0 35593-13-6

RL: RCT (Reactant)
 (addn. reaction of, with nucleophiles)

IT 67-56-1, reactions 107-21-1, reactions

RL: RCT (Reactant)
 (addn., with .beta.-haloenamines)

IT 14865-53-3P 23588-56-9P 25386-76-9P 30269-19-3P 30269-20-6P
 34683-59-5P 39618-73-0P 39618-74-1P 57559-13-4P 57559-15-6P
 57559-16-7P 57559-17-8P 57559-18-9P 57559-19-0P 57559-20-3P
 57559-21-4P 57559-22-5P 57559-23-6P 57559-24-7P 57559-25-8P
 57579-03-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 75-08-1

RL: RCT (Reactant)
 (reaction of, with .beta.-haloenamines)

IT 16826-16-7

RL: RCT (Reactant)
 (reaction of, with bromine)

IT 57559-14-5

RL: RCT (Reactant)
 (reaction of, with methanol)

IT 7726-95-6, reactions

RL: RCT (Reactant)
 (with (diethylamino)isobutene)

L199 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1975:16254 HCAPLUS

DN 82:16254

TI .alpha.-Chloroenamines. New
 reagents for organic synthesis

AU Ghosez, Leon

CS Lab. Chim. Org. Synth., Univ. Cathol. Louvain, Louvain, Belg.

SO Angew. Chem., Int. Ed. Engl. (1972), 11(9), 852-3

CODEN: ACIEAY

DT Journal

LA English

CC 23-4 (Aliphatic Compounds)

Section cross-reference(s): 27

GI For diagram(s), see printed CA Issue.

AB R1CR2:CC1NR3R4 (I; R1 = alkyl, aryl, H2C:CH; R2 = H, alkyl; R3, R4 =
 alkyl, cycloalkyl), with an electron donating group and a suitable leaving
 group on a sp2 C had versatile chem. behavior. I reacted with N3- via
 R1CR2:-C:N+R3R4 (II) to give azirines III. Reaction of furan or pyrrole
 with II resulted in aminoalkenylation to give IV (X = O, NH). Reaction of
 II with H2C:CH2 gave high yields of cyclobutanes V. I reacted with Br
 (followed by H2O) to give R1CR2BrCONR3R4. Reaction of I with Mg gave
 R1CR2:C(MgCl)NR3R4 which were hydrolyzed to R1CR2:CHNR3R4 or were coupled
 with I to give R1CR2:C(NR3R4)C(NR3R4):CR1R2.

ST chloroenamine; enamine chloro; vinylamine
 chloro; azirine amino; furan aminovinyl; pyrrolidine aminovinyl

IT Alkenes, reactions

RL: RCT (Reactant)
 (with chloroenamines)

IT Ethenamine, 1-chloro-, derivs.

RL: RCT (Reactant)
 (new reagents for org. synthesis)

IT Ethenamine, magnesium complex, derivs.

Magnesium, (1-aminoethenyl)chloro-, derivs.

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reactions of)

IT 1,3-Butadiene-2,3-diamine, derivs.

2-Furanmethanamine, .alpha.-methylene-, derivs.
Acetamide, 2-bromo-, derivs.

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT Ethenimine, derivs.

RL: RCT (Reactant)
(reactions of)

IT 54786-32-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 110-00-9 123-75-1 54376-55-5 54376-56-6

RL: RCT (Reactant)
(reaction of, with chloroenamines)

IT 74-85-1, reactions

RL: RCT (Reactant)
(with chloroenamines, cyclobutanes from)

L199 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1974:437309 HCAPLUS

DN 81:37309

TI Chemistry of small ring compounds. 24. Improved synthesis of amins of bicyclo[3.1.0]hexan-6-one and bicyclo[4.1.0]heptan-7-one

AU Jongejan, E.; Steinberg, H.; De Boer, Th. J.

CS Lab. Org. Chem., Univ. Amsterdam, Amsterdam, Neth.

SO Syn. Commun. (1974), 4(1), 11-16

CODEN: SYNCAV

DT Journal

LA English

CC 24-7 (Alicyclic Compounds)

GI For diagram(s), see printed CA Issue.

AB **Enamines** (I; n = 1,2) were prepd. in 85 and 82% yield, resp., by reaction of .alpha.-bromocyclohexanone and -cycloheptanone with Me₂NH and TiCl₄. Reaction of I with a Me₂NH-AgBF₄ complex gave the corresponding amins (II) in almost quant. yield.

ST bicyclohexanone amina; bicycloheptanone amina; cycloalkanone
enamine cyclization

IT **Amines**, preparation

RL: PREP (Preparation)
(enamines, cyclic .alpha.-halo)

IT Amins

RL: RCT (Reactant)
(of bicyclohexanone and bicycloheptanone)

IT 52999-06-1P 52999-07-2P 52999-08-3P 52999-09-4P 52999-11-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 766-65-4

RL: RCT (Reactant)
(reaction of, with dimethylamine and titanium **chloride**)

IT 822-85-5

RL: RCT (Reactant)
(reaction of, with dimethylamine and titanium **chloride**,
enamine from)

IT 124-40-3, reactions

RL: RCT (Reactant)
(with **bromocycloheptanone** and titanium **chloride**,
enamine from)

IT 7550-45-0, reactions

RL: RCT (Reactant)
(with dimethylamine and **bromocycloheptanone**, **enamine**
from)

L199 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1974:47377 HCAPLUS

- DN 80:47377
TI Action of **halogens** on **enamines** and **.beta.-halo enamines**. Route to **.beta.-halo enamines** and **.alpha.,.alpha.-dihalo aldehydes**
AU Duhamel, Lucette; Duhamel, Pierre; Poirier, Jean M.
CS Lab. Chim. Org., Fac. Sci. Tech. Rouen, Mont-Saint-Aignan, Fr.
SO Tetrahedron Lett. (1973), (43), 4237-40
CODEN: TELEAY
DT Journal
LA French
CC 23-4 (Aliphatic Compounds)
AB The **.beta.-halo enamines** RR1C:CR2R3 (R = Et, R1 = Cl, R2 = H, R3 = NEt2; R = H, R1 = Cl, Br, R2 = CMe3, R3 = morpholino) were prepd. from RCH:CR2R3 by reaction with **halogen** and treatment of the **.alpha.-halo immonium halide** with NEt3. RR1C:CHR2 [R = Et, R1 = Cl, R2 = NEt; R = (CH2)4Me, CMe3, R1 = Cl, R2 = morpholino; R = CMe3, R1 = Br, R2 = piperidino] with **halogen** gave **.alpha.,.alpha.-dihalo immonium salts** which hydrolyzed to RCR1R2CHO [R = Et, CMe3, R1 = Cl, R2 = Cl, Br; R = (CH2)4Me, R1 = R2 = Cl; R = CMe3, R1 = R2 = Br].
ST **enamine halo; halo aldehyde; halogen addn enamine**
IT 15430-99-6 22502-84-7 27971-18-2 35593-10-3
RL: RCT (Reactant)
(halogenation of)
IT 1937-09-3P 22518-16-7P 23454-01-5P 34342-17-1P 35593-04-5P
50735-71-2P 51042-97-8P 51042-98-9P 51094-53-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 7726-95-6, reactions 7782-50-5, reactions
RL: RCT (Reactant)
(with **enamines** and **.beta.-haloenamines**)

L199 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:514325 HCAPLUS
DN 77:114325
TI **.alpha.-Halogenated amines**. 44. Reaction of **enamines** with dialkylmethyleniminium halides
AU Boehme, Horst; Osmers, Knut; Wagner, Peter
CS Pharm.-Chem. Inst., Univ. Marburg/Lahn, Marburg/Lahn, Ger.
SO Tetrahedron Lett. (1972), (27), 2785-6
CODEN: TELEAY
DT Journal
LA German
CC 28-14 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27, 22
AB Morpholinopivalaldehyde (I) was obtained by treating N-(**chloromethyl**)morpholine (II) with 1-morpholinoisobutene (III), N-(**chloromethyl**)piperidine with III, or II with 1-piperidinoisobutene and hydrolysis. The intermediate iminium salt (R2NCH2CMe2CH:NR21+Cl-, R2N = piperidino, R21N = morpholino) underwent an intramol. hydride shift to R21NCH2CMe2CH:NR2+Cl-, which was hydrolyzed to I.
ST **enamine** iminium halide addn; morpholinopivalaldehyde
IT **Amines**, reactions
Amines, reactions
RL: RCT (Reactant)
(**enamines**, with dialkylmethyleniminium halides)
IT Methanimine, quaternary halides
RL: RCT (Reactant)
(reaction of, with **enamines**)
IT Methanimine, quaternary derivs.
RL: RCT (Reactant)
(reaction with **enamines**)

- IT 23588-51-4P 37591-27-8P 37810-60-9P 37810-63-2P 37810-64-3P
37810-65-4P 37810-66-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 2403-55-6
RL: RCT (Reactant)
(reaction with **chloromethylamines**)
- IT 673-33-6
RL: RCT (Reactant)
(reaction with **chloromethylmorpholine**)
- IT 16158-87-5 16158-88-6
RL: RCT (Reactant)
(reaction with morpholinoisobutene)
- L199 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:113145 HCAPLUS
DN 76:113145
TI **.beta.-Halo enamines**. Synthesis from **.alpha**
.-chloro-, .alpha.-bromo-, or .alpha
.-iodoaldehydes
- AU Duhamel, Lucette; Duhamel, Pierre; Poirier, Jean M.
CS Lab. Chim. Org., Fac. Sci. Rouen, Mont-Saint-Aignan, Fr.
SO Bull. Soc. Chim. Fr. (1972), (1), 221-6
CODEN: BSCFAS
DT Journal
LA French
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27, 23
- AB Twenty-five **.beta.-halo enamines** RC(X):CHNR12 [R = Et, n-pentyl, Me2CCH2, Me3C; X = Cl, Br, I; NR12 = NEt2, NPr2, piperidino, morpholino, 1-pyrrolidinyl, NMe2, N(Me)Ph] were prepd. by treatment of **.beta.-haloaldehydes** with As(NR12)3 or with AsCl3, SbCl3, BiCl3, AlCl3 or TiCl4 in the presence of a secondary amine. A soln. of triperidinoarsine in anhyd. benzene was added dropwise to a soln. of 2-**chlorobutanal** in Et2O at 5-10.degree. and the mixt. stirred 0.5 hr and kept overnight at -30.degree. to give 2-**chloro**-1-piperidino-1-butene. A soln. of Et2NH in Et2O was added to a mixt. of 2-**bromoneohexanal** in anhyd. Et2O and AsCl3 in anhyd. benzene at 5-10.degree. and the mixt. stirred 0.5 hr and kept overnight at 30.degree. to give 2-**bromo**-1-diethylamino-3,3-dimethyl-1-butene.
- ST **enamine halo**
IT **Amines**, preparation
RL: PREP (Preparation)
(**enamines**, from **haloaldehydes**)
- IT Aldehydes, reactions
RL: SPN (Synthetic preparation); PREP (Preparation)
(**halo**, prepn. of **halo enamines** from)
- IT 27971-16-0P 27971-17-1P 27971-18-2P 27971-19-3P 27971-20-6P
27971-21-7P 27971-22-8P 27971-23-9P 27971-24-0P 27974-33-0P
35593-04-5P 35593-05-6P 35593-06-7P 35593-07-8P 35593-08-9P
35593-09-0P 35593-10-3P 35593-11-4P 35593-12-5P 35593-13-6P
35593-14-7P 35593-15-8P 35593-16-9P 35593-17-0P 35593-19-2P
35593-20-5P 35593-21-6P 35593-22-7P 35593-23-8P 35593-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 35593-18-1
RL: RCT (Reactant)
(prepn. of **halo enamines** from)

L199 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:99016 HCAPLUS
DN 76:99016
TI **.alpha.-Halo immonium salts**. Preparation from .

alpha.-halo enamines. Action of primary,
secondary, and **tertiary amines**

- AU Duhamel, Pierre; Duhamel, Lucette; Poirier, Jean M.
CS Lab. Chim. Org., Fac. Sci. Rouen, Mont-Saint-Aignan, Fr.
SO C. R. Acad. Sci., Ser. C (1972), 274(4), 411-14
CODEN: CHDCAQ
DT Journal
LA French
CC 23 (Aliphatic Compounds)
AB **Enamines** RCX:CHNR21 (R = tert-Bu, Et, X = Cl, Br, R21N = Me2N, Et2N, morpholino, or piperidino) were titrated with HClO4 in HOAc or HCl in Et2O to give RCHXCH:N+R21Z- (Z = ClO4 or Cl). These reacted with iso-PrNH2 to give the original **enamine**, and reacted with secondary amines HNR22 (pyrrolidine, piperidine, morpholine, Et2NH, or Pr2NH) to give RC:-CHNR22.
- ST **enamines** prepn immonium salts; immonium salt reaction amine; morpholine **enamines**; pyrrolidine **enamines**; piperidine **enamines**; halo immonium salt **enamine**
- IT **Amines**, reactions
RL: RCT (Reactant)
(with aliphatic and heterocyclic **halo** immonium salts)
- IT 34683-43-7P 34683-58-4P 34683-59-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 75-31-0 108-91-8 110-91-8 142-84-7
RL: RCT (Reactant)
(reaction of, with aliphatic and heterocyclic **halo** immonium salts)
- IT 123-75-1
RL: RCT (Reactant)
(reaction of, with aliphatic heterocyclic **halo** immonium salts)
- IT 34683-46-0 34683-47-1 34683-48-2 34683-49-3 34683-50-6
34683-51-7 34683-52-8 34683-53-9 34683-54-0 34683-55-1
34683-56-2 34683-57-3
RL: RCT (Reactant)
(reaction of, with amines)
- IT 109-89-7, reactions 110-89-4, reactions
RL: RCT (Reactant)
(with aliphatic and heterocyclic **halo** immonium salts)
- L199 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1972:25205 HCAPLUS
DN 76:25205
TI Reactions and mechanisms of **.alpha.-haloenamine**
AU Hsu, Eric T. H.
CS Univ. Connecticut, Storrs, Conn., USA
SO (1971) 104 pp. Avail.: Univ. Microfilms, Ann Arbor, Mich., Order No. 71-18,415
From: Diss. Abstr. Int. B 1971, 32(1), 168
DT Dissertation
LA English
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
AB Unavailable
ST **halo enamine**; morpholino diphenylethene
IT **Amines**, reactions
RL: RCT (Reactant)
(**enamines**, **.alpha.-halo**)
- IT Reaction mechanism
(of **.alpha.-haloenamines**)

L199 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1971:3771 HCAPLUS

DN 74:3771
TI Functionalized **enamines**. IX. Synthesis of fused furan systems
via reaction of conjugated **enamines** with **.alpha.-haloketones**
AU Pandit, Upendra K.; Reus, H. R.; De Jonge Mrs. K.
CS Lab. Org. Chem., Univ. Amsterdam, Amsterdam, Neth.
SO Recl. Trav. Chim. Pays-Bas (1970), 89(9), 956-60
CODEN: RTCPA3
DT Journal
LA English
CC 32 (Steroids)
GI For diagram(s), see printed CA Issue.
AB Re-action of conjugated **enamines** with **.alpha.-bromoketones** in DMF leads to the formation of substituted furans
in one practical step. The reaction has been applied to the synthesis of
steroido-[3,4-b]furans, e.g. I.
ST furans steroids; **enamines bromoketones** reactions;
naphthalenes furans
IT Ketones, reactions
RL: RCT (Reactant)
(**.alpha.-halo**, with conjugated **enamines**)
IT **Amines**, reactions
RL: RCT (Reactant)
(**enamines, .alpha.-haloketones** with
conjugated)
IT Androsta-3,5-dieno[3,4-b]furan-17.beta.-ol, 5'-ethyl-, acetate
Androsta-3,5-dieno[3,4-b]furan-17.beta.-ol, 5'-phenyl-, acetate
Cyclohexanone, 2-(2-oxobutyl)-
Inden-2(4H)-one, 5,6,7,7a-tetrahydro-3-methyl-
Naphtho[2,1-b]furan-6(4H)-one, 2-ethyl-5,5a,7,8-tetrahydro-5a-methyl-
Naphtho[2,1-b]furan-6(4H)-one, 5,5a,7,8-tetrahydro-2-(m-methoxyphenyl)-5a-
methyl-
Naphtho[2,1-b]furan-6(4H)-one, 5,5a,7,8-tetrahydro-5a-methyl-2-phenyl-
Pregna-3,5,7-trieno[3,4-b]furan-20-one, 5'-phenyl-
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L199 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1970:444522 HCAPLUS
DN 73:44522
TI Synthesis and reactions of mono **.alpha.-halo enamines**
AU Lessard, Marie V.
CS Univ. of Connecticut, Storrs, Conn., USA
SO (1969) 131 pp. Avail.: 70-1281
From: Diss. Abstr. Int. B 1970, 30(7), 3099-100
DT Dissertation
LA English
CC 22 (Physical Organic Chemistry)
AB Unavailable
ST **enamines halogenated; halogenated enamines**
IT **Amines**, preparation
RL: PREP (Preparation)
(**enamines, mono .alpha.-halo**)

L199 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2002 ACS
AN 1969:480614 HCAPLUS
DN 71:80614
TI **.alpha.-Chloroenamines**. III. Substitution and
elimination reactions on **.alpha.-chloroenamine**
-**.beta.-acid** derivatives. The synthesis of an **ynamine**
amide and an **ynamine** ester

AU Buyle, R.; Viehe, Heinz G.
CS Union Carbide Eur. Assoc. Res., Brussels, Belg.
SO Tetrahedron (1969), .25(16), 3447-51
CODEN: TETRAB
DT Journal
LA English
CC 23 (Aliphatic Compounds)
AB Readily accessible .beta.-chloroacyl-.alpha.-
chloro enamines have two reactive Cl atoms which can be
substituted successively with nucleophilic reagents. MeO2CC.tplbond.CNEt2
and Et2NCOC.tplbond.CNEt2 were prepd. from N,N-diethylchloroacetamide via
its .beta.-chloro-.beta.-chloroacyl-.alpha.-
chloro enamine by **chlorine** elimination with Li
amalgam.
ST **chloro enamines**; **enamines chloro**;
ynamine amides; amides ynamine; esters ynamines
IT Acid **chlorides**
RL: RCT (Reactant)
(aminoalkene, reaction of)
IT 17691-75-7P 25491-79-6P 25491-80-9P 25491-81-0P 25491-82-1P
25491-83-2P 25491-84-3P 25491-85-4P 25491-86-5P
25492-14-2P 25503-08-6P 25542-59-0P 25542-60-3P
25542-61-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L199 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1969:438880 HCAPLUS

DN 71:38880

TI Alkyl and aryl .alpha.-chloro
enamines

AU Ghosez, Leon; Haveaux, B.; Viehe, H. G.

CS Univ. Cath. Louvain, Louvain, Belg.

SO Angew. Chem., Int. Ed. Engl. (1969), 8(6), 454-5

CODEN: ACIEAY

DT Journal

LA English

CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

AB R1R2CHCONR2, where R is Et and NR2 is piperidino and morpholino, are
treated with COCl2 and base (Et3N or pyridine) to give **chloro**
enamines R1R2C:CClNR2 (I). Nucleophilic substitution reactions of
I (R1 = R2 = Me, NR2 = piperidino) with R3M, where R3 is Me, Ph, EtS, EtO,
and cyclohexyl and M is Li, Na, and MgBr, give Me2C:CR3NR2.

ST **enamines**; piperidines; morpholines; amines unsatd; unsatd amines

IT **Amines**, preparation

RL: PREP (Preparation)

(enamines, chloro).

IT 23150-97-2P 23150-98-3P 23150-99-4P

23151-00-0P 23151-01-1P 23151-02-2P 23257-81-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L199 ANSWER 35 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1968:114025 HCAPLUS

DN 68:114025

TI .alpha.-Chloroenamines. I. Acylation of
ynamines

AU Buyle, Raoul; Viehe, Heinz G.

CS Union Carbide Eur. Res. Assoc., Brussels, Belg.

SO Tetrahedron (1968), 24(10), 3987-95

CODEN: TETRAB

DT Journal

LA French

- CC 23 (Aliphatic Compounds)
 GI For diagram(s), see printed CA Issue.
 AB Acid **chlorides**, phosgene, thiophosgene, SOCl₂ and aromatic sulfonyl **chlorides** readily add to ynamines to give .**alpha.-chloroenamines**. The .**alpha.-chloro-.beta.-chlorocarbonylenamines** are thermally remarkably stable as illustrated by their distn. in vacuo without decompn. The reaction of ynamines with oxalyl **chloride** led to 5-(disubstituted amino)-2,2-dichloro-2,3-dihydro-3-furanones (I). The structure of these .**alpha.-chloroenamines** was established by hydrolysis, alcoholysis, and aminolysis.
- ST YNAMINES ACYLATION **ENAMINES** VIA; **ENAMINES** VIA ACYLATION YNAMINES
- IT **Amines**, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (enamines, .**alpha.-chloro**, prepn. by ynamine acylation, and reactions thereof)
- IT Addition reactions
 (of ynamines with acid **chlorides**, .**alpha.-chloro enamines** by)
- IT Acylation
 (of ynamines, .**alpha.-chloro enamines** by)
- IT Acid **chlorides**
 RL: RCT (Reactant)
 (reactions of, with ynamines, .**alpha.-chloro enamines** by)
- IT 4647-28-3P 14110-41-9P 14110-43-1P 14110-49-7P
 19698-32-9P 20251-21-2P 20251-24-5P 20251-25-6P
 20251-26-7P 20251-27-8P 20251-28-9P 20251-29-0P 20251-30-3P
 20251-31-4P 20251-32-5P 20251-33-6P 20251-34-7P 20251-35-8P
 20251-36-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- L199 ANSWER 36 OF 37 HCAPLUS COPYRIGHT 2002 ACS
 AN 1967:402946 HCAPLUS
 DN 67:2946
 TI Cyclic **enamines** and imines
 AU Blaha, Karel; Cervinka, Otakar
 CS Inst. Org. Chem. Biochem., Prague, Czech.
 SO Advan. Heterocycl. Chem. (1966), 6, 147-227
 DT Journal
 LA English
 CC 27 (Heterocyclic Compounds (One Hetero Atom))
 AB Compds. contg. an **enamine** group (-N=C:C-) in which at least the N atom is part of a ring are reviewed with 416 references. Discussed are structure and physicochem. properties, differences in structure and properties of secondary **enamines** and tertiary **enamines**, and the phenomena of pseudobases and transannular interactions; prepn. of **enamines** by condensation of aldehydes and ketones with amines; prepn. by redn. methods (e.g., partial hydrogenation of quaternary pyridine salts in strongly alk. media, redn. of N-methylpyrrolidone with LiAlH₄, redn. of N-alkypiperidones with Na in EtOH, etc.); prepn. by means of organometallic reagents (e.g., treatment of .gamma.-**halo** and .delta.-**halo** nitriles with Grignard reagents to form 1-pyrrolines and 1-piperideines, reaction of N-methyl lactams with Grignard reagents, treatment of imino ethers with Grignard reagents); prepn. utilizing the Claisen condensation (condensation of the .**alpha.-methylene** group in lactams with esters of formic, oxalic, and arylcarboxylic acids); prepn. by elimination reactions (e.g., dehydrohalogenation of N-**chloropyrrolidine** and N-**chloropiperidine** to form 1-pyrroline and 1-piperideine, enzymic oxidative deamination, dehydrogenation of satd. bases with Hg(OAc)₂ as in

the dehydrogenation of yohimbine or of 1-methyl-1-azacyclooctane); prepn. by special methods (e.g., pyrolysis of azidostyrene to form a cyclic imine with a 3-membered ring; and reactions of **enamines** with electrophilic and nucleophilic reagents, aldol reactions, special reactions of heteroaromatics contg. an imine group.

IT **Amines**, preparation

Amines, properties.

RL: PRP (Properties)

(**enamines**, cyclic)

L199 ANSWER 37 OF 37 HCAPLUS COPYRIGHT 2002 ACS

AN 1960:2261 HCAPLUS

DN 54:2261

OREF 54:541i,542a-f

TI **.alpha.-Halogenated amines**. VI. The cleavage of amins of higher aldehydes with hydrogen halides and the addition of hydrogen **chloride** to **enamines**

AU Bohme, Horst; Ellenberg, Horst; Herboth, Otto E.; Lehnert, Walter

CS Univ. Marburg, Germany

SO Chem. Ber. (1950), 92, 1608-13

DT Journal

LA Unavailable

CC 10G (Organic Chemistry: Heterocyclic Compounds)

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 52, 13726d. The cleavage of amins of aliphatic or aromatic aldehydes with hydrogen halides yielded the corresponding **.alpha.-halogenated amines** of the type $RCHClNR_2$ which were also obtained by the reaction of **enamines** with hydrogen halides. HCl (3.0 g.) in 25 cc. MeCN added dropwise at -15.degree. to 9.5 g. N,N'-benzylidenedimorpholine in 30 cc. MeCN and 20 cc. Et2O, filtered, and evapd. yielded 8.2 g. N-(**.alpha.-chlorobenzyl**)morpholine (I). I (9.0 g.) in dry Et2O treated with cooling with 1 equiv. PhLi in Et2O, refluxed 0.5 hr., cooled, dild. with iced H2O, and extd. with Et2O, the ext. reextd. with dil. acid, the aq. acidic ext. basified and extd. with Et2O, and the Et2O evapd. yielded 5.2 g. N-benzhydrylmorpholine, b0.01 90-100.degree. (bath); HCl salt m. 230-3.degree. (iso-PrOH-Et2O). N,N'-Benzylidenedipiperidine (10 g.) in 50 cc. Et2O added dropwise to 3.7 g. HCl in 25 cc. MeCN, filtered, and evapd. in vacuo, the residue treated with cooling with HCN, the excess HCN removed in vacuo, the residue dissolved in H2O, and treated with aq. KOH, and the product isolated with Et2O gave 4.9 g. N-(**.alpha.-cyanobenzyl**)piperidine, b0.5 112.degree., m. 62.degree.; picrate m. 141.degree. (Et2O). Isobutyraldehyde tetramethylaminal, $Me_2CHCH(NMe_2)_2$ (4.0 g.), b10 39.5-41.0.degree., in 40 cc. Et2O added (at -15.degree.) dropwise to 2.2 g. HCl in dry Et2O pptd. 6.0 g. mixt. of 44% **.alpha.-haloamine** and 56% $Me_2NH.HCl$; a 4-g. portion of the mixt. dissolved in 30 cc. HCN and worked up as usual gave 1.5 g. $Me_2NCH(CN)CHMe_2$, b10 54.degree.. **.alpha.-Tripiperidine** (II) (7.0 g.) in Et2O treated with cooling with 3 equivs. HCl in Et2O and filtered gave 8.0 g. III. The III treated with 30 cc. liquid HCN gave in the usual manner 7.0 g. 2-cyanopiperidine (IV), b12 90-2.degree.; picrate m. 134.degree. (EtOH-petr. ether); IV.HCl m. 138.degree. (EtOH-petr. ether). II (2.8 g. treated with cooling with 20 cc. HCN yielded 3.0 g. IV, b9 82-4.degree.. IV (1.5 g.) heated with 5.0 g. $Ba(OH)_2$ in 30 cc. H2O until the NH_3 odor had disappeared, and the product isolated with Et2O gave 2-carboxypiperidine, m. 262.degree.. II (7.0 g.) and 8.0 g. III in 50 cc. Et2O treated with stirring and cooling with an equiv. amt. PhLi in Et2O, stored 12 hrs., and worked up as usual gave 5.3 g. 2-phenylpiperidine, b13 118.degree., which in air formed the hydrate, m. 60.degree.; HCl salt m. 195-6.degree.. 1-Morpholino-1-butene (12.0 g.) in 30 cc. Et2O treated dropwise at -15.degree. with 3.1 g. HCl in dry Et2O and filtered, the residue dried and dissolved in HCN, and the mixt. worked up gave 6.0 g. **.alpha.-morpholinovaleronitrile** (V), b15

134-6.degree., m. 32.degree.; V.HCl, m. 148.degree. (EtOH-petr. ether).
 1,1-Dimorpholinobutane (20.0 g.) and 6.4 g. HCl in dry Et2O deposited at
 -15.degree. 15.8 g. mixt. of 37% **.alpha.-haloamine** and
 63% morpholine-HCl; a 14.0-g. portion of the mixt. treated with HCN gave
 4.5 g. V, b15 134-6.degree., m. 32.degree.; V.HCl, m. 148.degree..

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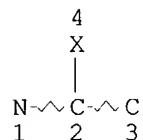
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 in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que 188

L84 STR



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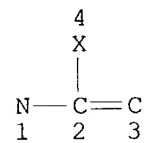
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L86 25524 SEA FILE=REGISTRY SSS FUL L84
 L87 STR



NODE ATTRIBUTES:

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 NSPEC IS RC AT 3

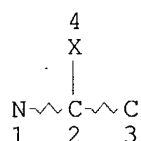
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 DEFAULT ECLEVEL IS LIMITED

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 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE
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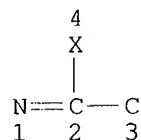
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 L84 STR



NODE ATTRIBUTES:
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 NSPEC IS RC AT 3
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE
 L86 25524 SEA FILE=REGISTRY SSS FUL L84
 L89 STR



NODE ATTRIBUTES:
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

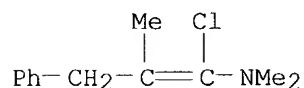
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 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE
 L90 10183 SEA FILE=REGISTRY SUB=L86 SSS FUL L89

100.0% PROCESSED 10183 ITERATIONS 10183 ANSWERS
 SEARCH TIME: 00.00.01

=> d ide can 1123

L123 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN 124805-03-4 REGISTRY
 CN 1-Propen-1-amine, 1-chloro-N,N,2-trimethyl-3-phenyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C12 H16 Cl N
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT



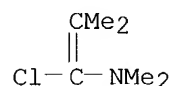
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:55680

=> d ide can 1121

L121 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN 26189-59-3 REGISTRY
 CN 1-Propen-1-amine, 1-chloro-N,N,2-trimethyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Propenylamine, 1-chloro-N,N,2-trimethyl- (8CI)
 OTHER NAMES:
 CN 1-Chloro-1-(dimethylamino)-2-methylpropene
 CN 1-Chloro-N,N-2-trimethylpropenylamine
 FS 3D CONCORD
 MF C6 H12 Cl N
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSChem, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

71 REFERENCES IN FILE CA (1967 TO DATE)
 71 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:279242

REFERENCE 2: 136:200113

REFERENCE 3: 135:288703

REFERENCE 4: 134:311379

REFERENCE 5: 129:216202

REFERENCE 6: 128:283012
REFERENCE 7: 128:217218
REFERENCE 8: 128:114953
REFERENCE 9: 128:114663
REFERENCE 10: 127:162122

=> d ide can 1131

L131 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 77716-11-1 REGISTRY

CN 1H-Pyrrole-2-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)

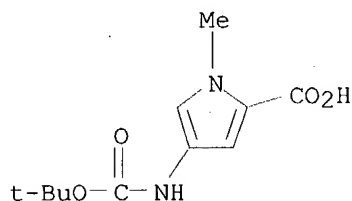
FS 3D CONCORD

MF C11 H16 N2 O4

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

23 REFERENCES IN FILE CA (1967 TO DATE)

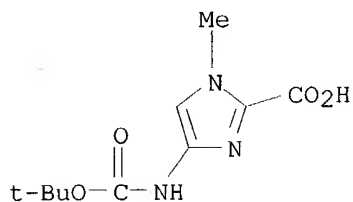
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

23 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 137:169795
REFERENCE 2: 136:85750
REFERENCE 3: 136:54024
REFERENCE 4: 136:1626
REFERENCE 5: 135:353702
REFERENCE 6: 135:298753
REFERENCE 7: 133:223039
REFERENCE 8: 132:22791
REFERENCE 9: 132:19609
REFERENCE 10: 130:14267

=> d ide can 1177

L177 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 128293-64-1 REGISTRY
CN 1H-Imidazole-2-carboxylic acid, 4-[[[1,1-dimethylethoxy]carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H15 N3 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



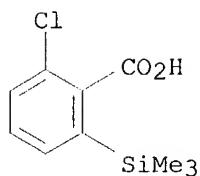
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

20 REFERENCES IN FILE CA (1967 TO DATE)
20 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:54024
REFERENCE 2: 136:1626
REFERENCE 3: 135:46422
REFERENCE 4: 135:5798
REFERENCE 5: 134:233190
REFERENCE 6: 134:207755
REFERENCE 7: 134:26617
REFERENCE 8: 133:335106
REFERENCE 9: 133:223039
REFERENCE 10: 132:118894

=> d ide can 1134

L134 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 150079-25-7 REGISTRY
CN Benzoic acid, 2-chloro-6-(trimethylsilyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H13 Cl O2 Si
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

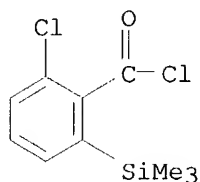
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:145558

REFERENCE 2: 119:160256

=> d ide can 1136

L136 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 150079-26-8 REGISTRY
CN Benzoyl chloride, 2-chloro-6-(trimethylsilyl)- (9CI) (CA INDEX
NAME)
FS 3D CONCORD
MF C10 H12 Cl2 O Si
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



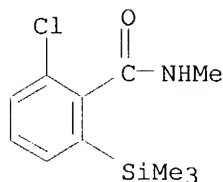
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:160256

=> d ide can 1158

L158 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 150108-45-5 REGISTRY
CN Benzamide, 2-chloro-N-methyl-6-(trimethylsilyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H16 Cl N O Si
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:160256

=> d ide can 1140

L140 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 69-72-7 REGISTRY

CN **Benzoic acid, 2-hydroxy- (9CI)** (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Salicylic acid (6CI, 8CI)

OTHER NAMES:

CN 2-Carboxyphenol

CN 2-Hydroxybenzenecarboxylic acid

CN 2-Hydroxybenzoic acid

CN o-Carboxyphenol

CN o-Hydroxybenzoic acid

CN Phenol-2-carboxylic acid

CN Psoriacid-S-Stift

CN Retarder W

CN Rutranex

CN Salicylic acid collodion

CN Salonil

FS 3D CONCORD

DR 7681-06-3, 8052-31-1

MF C7 H6 O3

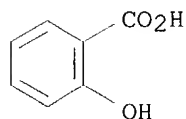
CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSChem, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16734 REFERENCES IN FILE CA (1967 TO DATE)
2208 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
16777 REFERENCES IN FILE CAPLUS (1967 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:178980
REFERENCE 2: 137:177341
REFERENCE 3: 137:176992
REFERENCE 4: 137:175110
REFERENCE 5: 137:175083
REFERENCE 6: 137:174728
REFERENCE 7: 137:174687
REFERENCE 8: 137:174546
REFERENCE 9: 137:174545
REFERENCE 10: 137:172189

=> d ide can l143

L143 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 1441-87-8 REGISTRY

CN Benzoyl chloride, 2-hydroxy- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Salicyloyl chloride (6CI, 7CI, 8CI)

OTHER NAMES:

CN 2-Hydroxybenzoyl chloride

CN o-Hydroxybenzoyl chloride

CN Salicyl chloride

CN Salicylic acid chloride

FS 3D CONCORD

MF C7 H5 Cl O2

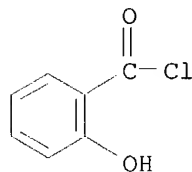
CI COM

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
CHEMINFORMRX, CHEMLIST, HODOC*, IFICDB, IFIPAT, IFIUDB, TOXCENTER,
USPATFULL

(*File contains numerically searchable property data)

Other Sources: EINECS**

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

182 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

182 REFERENCES IN FILE CAPLUS (1967 TO DATE)
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:340997
REFERENCE 2: 135:288742
REFERENCE 3: 135:242175
REFERENCE 4: 134:366835
REFERENCE 5: 134:340466
REFERENCE 6: 134:280845
REFERENCE 7: 134:46644
REFERENCE 8: 133:317397
REFERENCE 9: 133:150124
REFERENCE 10: 132:347588

=> d ide can 1146

L146 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 119-36-8 REGISTRY

CN Benzoic acid, 2-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Salicylic acid, methyl ester (6CI, 8CI)

OTHER NAMES:

CN 2-(Methoxycarbonyl)phenol

CN 2-Carbomethoxyphenol

CN 2-Hydroxybenzoic acid methyl ester

CN Analgit

CN Anthrapole ND

CN Exagien

CN Flucarmit

CN Methyl 2-hydroxybenzoate

CN Methyl o-hydroxybenzoate

CN Methyl salicylate

CN o-Hydroxybenzoic acid methyl ester

CN Wintergreen oil

FS 3D CONCORD

DR 8022-86-4, 8024-54-2

MF C8 H8 O3

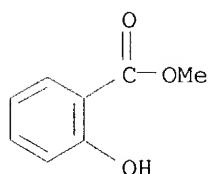
CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PHARMASEARCH, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3459 REFERENCES IN FILE CA (1967 TO DATE)
 78 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 3469 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 115 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:171357
 REFERENCE 2: 137:169470
 REFERENCE 3: 137:154948
 REFERENCE 4: 137:152349
 REFERENCE 5: 137:152311
 REFERENCE 6: 137:151347
 REFERENCE 7: 137:140331
 REFERENCE 8: 137:139672
 REFERENCE 9: 137:129863
 REFERENCE 10: 137:124335

=> d ide can l148

L148 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 99-96-7 REGISTRY

CN Benzoic acid, 4-hydroxy- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzoic acid, p-hydroxy- (8CI)

OTHER NAMES:

CN 4-Carboxyphenol

CN 4-Hydroxybenzoic acid

CN p-Carboxyphenol

CN p-Hydroxybenzoic acid

CN p-Salicylic acid

CN Paraben-acid

FS 3D CONCORD

MF C7 H6 O3

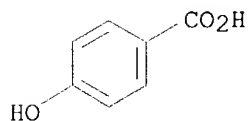
CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU, EMBASE, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8012 REFERENCES IN FILE CA (1967 TO DATE)
702 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
8027 REFERENCES IN FILE CAPLUS (1967 TO DATE)
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:178864
REFERENCE 2: 137:173993
REFERENCE 3: 137:171357
REFERENCE 4: 137:171220
REFERENCE 5: 137:169712
REFERENCE 6: 137:169287
REFERENCE 7: 137:168563
REFERENCE 8: 137:166271
REFERENCE 9: 137:166236
REFERENCE 10: 137:165748

=> d ide can l150

L150 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 28141-24-4 REGISTRY

CN Benzoyl chloride, 4-hydroxy- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzoyl chloride, p-hydroxy- (7CI)

OTHER NAMES:

CN 4-Hydroxybenzoyl chloride

CN p-Hydroxybenzoyl chloride

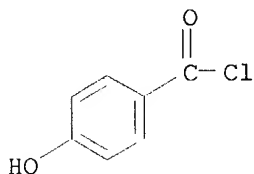
FS 3D CONCORD

MF C7 H5 Cl O2

CI COM

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT,
IFIUDB, TOXCENTER, USPATFULL

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

50 REFERENCES IN FILE CA (1967 TO DATE)
6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
50 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:136563
REFERENCE 2: 135:331243
REFERENCE 3: 135:84297
REFERENCE 4: 133:296035
REFERENCE 5: 133:281277
REFERENCE 6: 131:322448
REFERENCE 7: 129:343609
REFERENCE 8: 129:81542
REFERENCE 9: 127:325767
REFERENCE 10: 127:176727

=> d ide can l152

L152 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 99-76-3 REGISTRY

CN Benzoic acid, 4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzoic acid, p-hydroxy-, methyl ester (6CI, 8CI)

OTHER NAMES:

CN 4-(Carbomethoxy)phenol

CN 4-(Methoxycarbonyl)phenol

CN 4-Hydroxybenzoic acid methyl ester

CN E 218

CN E 218 (preservative)

CN Killitol

CN Maseptol

CN Mekkings M

CN Metaben

CN Metagin

CN Methaben

CN Methyl 4-hydroxybenzoate

CN Methyl Butex

CN Methyl chemosept

CN Methyl p-hydroxybenzoate

CN Methyl Parasept

CN Methylben

CN Methylparaben

CN Metoxyde

CN Moldex

CN Nipagin

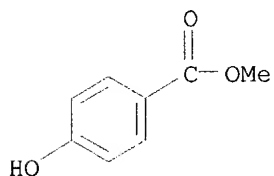
CN Nipagin M

CN p-Carbomethoxyphenol

CN p-Hydroxybenzoic acid methyl ester

CN p-Methoxycarbonylphenol

CN Para M
 CN Paridol
 CN Preserval
 CN Preserval M
 CN Septos
 CN Solbrol
 CN Solbrol M
 CN Tegosept M
 FS 3D CONCORD
 MF C8 H8 O3
 CI COM
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS,
 BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB,
 CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU,
 DETHERM*, DIOGENES, DRUGU, EMBASE, HODOC*, HSDB*, IFICDB, IFIPAT,
 IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PROMT,
 RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

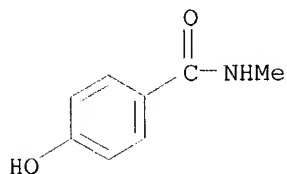
4129 REFERENCES IN FILE CA (1967 TO DATE)
 53 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 4140 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 170 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:174985
 REFERENCE 2: 137:174807
 REFERENCE 3: 137:174539
 REFERENCE 4: 137:171357
 REFERENCE 5: 137:166196
 REFERENCE 6: 137:165015
 REFERENCE 7: 137:161690
 REFERENCE 8: 137:159189
 REFERENCE 9: 137:159019
 REFERENCE 10: 137:145699

=> d ide can 1155

L155 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN 27642-27-9 REGISTRY

CN **Benzamide, 4-hydroxy-N-methyl-** (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN **Benzamide, p-hydroxy-N-methyl-** (7CI, 8CI)
 OTHER NAMES:
 CN **N-Methyl-p-hydroxybenzamide**
 CN **p-Hydroxy-N-methylbenzamide**
 FS 3D CONCORD
 MF C8 H9 N O2
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMLIST, IFICDB, IFIPAT,
 IFIUDB, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

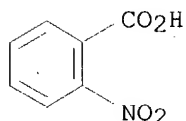
12 REFERENCES IN FILE CA (1967 TO DATE)
 12 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:37630
 REFERENCE 2: 124:316391
 REFERENCE 3: 117:69583
 REFERENCE 4: 112:189059
 REFERENCE 5: 89:122904
 REFERENCE 6: 85:143105
 REFERENCE 7: 85:4830
 REFERENCE 8: 72:111099
 REFERENCE 9: 65:29275
 REFERENCE 10: 61:54660

=> d ide can 1162

L162 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN **552-16-9** REGISTRY
 CN **Benzoic acid, 2-nitro-** (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN **Benzoic acid, o-nitro-** (8CI)
 OTHER NAMES:
 CN **2-Nitrobenzoic acid**
 CN **o-Carboxynitrobenzene**
 CN **o-Nitrobenzoic acid**
 FS 3D CONCORD

MF C7 H5 N O4
 CI COM
 LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHM, DETHERM*, EMBASE, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MSDS-OHS, NIOSHTIC, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1186 REFERENCES IN FILE CA (1967 TO DATE)
 16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1187 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:164866
 REFERENCE 2: 137:154661
 REFERENCE 3: 137:109401
 REFERENCE 4: 137:85356
 REFERENCE 5: 137:63215
 REFERENCE 6: 137:47439
 REFERENCE 7: 137:33054
 REFERENCE 8: 137:10200
 REFERENCE 9: 137:5892
 REFERENCE 10: 136:402022

=> d ide can l165

L165 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 610-14-0 REGISTRY

CN **Benzoyl chloride, 2-nitro- (9CI)** (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN **Benzoyl chloride, o-nitro- (7CI, 8CI)**

OTHER NAMES:

CN **2-Nitrobenzoyl chloride**

CN **o-Nitrobenzoic acid chloride**

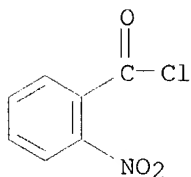
CN **o-Nitrobenzoyl chloride**

FS 3D CONCORD

MF **C7 H4 Cl N O3**

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHM, CSNB, GMELIN*, HODOC*, IFICDB, IFIPAT,

IFIUDB, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**, NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

525 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 525 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:169553
 REFERENCE 2: 137:125185
 REFERENCE 3: 137:125160
 REFERENCE 4: 137:125085
 REFERENCE 5: 137:109099
 REFERENCE 6: 137:93496
 REFERENCE 7: 137:79106
 REFERENCE 8: 137:78741
 REFERENCE 9: 137:59397
 REFERENCE 10: 137:47341

=> d ide can 1169

L169 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 606-27-9 REGISTRY

CN Benzoic acid, 2-nitro-, methyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzoic acid, o-nitro-, methyl ester (6CI, 7CI, 8CI)

OTHER NAMES:

CN 2-(Methoxycarbonyl)nitrobenzene

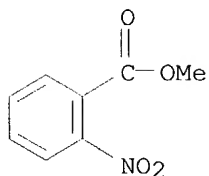
CN Methyl 2-nitrobenzoate

CN Methyl o-nitrobenzoate

FS 3D CONCORD

MF C8 H7 N O4

LC STN Files: ANABSTR, BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
 CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, HODOC*, IFICDB,
 IFIPAT, IFIUDB, MSDS-OHS, SPECINFO, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

102 REFERENCES IN FILE CA (1967 TO DATE)
 102 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:369322
 REFERENCE 2: 136:309702
 REFERENCE 3: 136:14981
 REFERENCE 4: 135:344257
 REFERENCE 5: 135:46170
 REFERENCE 6: 134:178126
 REFERENCE 7: 131:293348
 REFERENCE 8: 131:228273
 REFERENCE 9: 130:24998
 REFERENCE 10: 129:126769

=> d ide can 1172

L172 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 3400-29-1 REGISTRY

CN **Benzamide, N-methyl-2-nitro- (9CI)** (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN **Benzamide, N-methyl-o-nitro- (7CI, 8CI)**

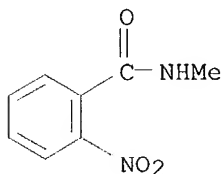
OTHER NAMES:

CN **N-Methyl-o-nitrobenzamide**

FS 3D CONCORD

MF **C8 H8 N2 O3**

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, USPATFULL
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1967 TO DATE)
 9 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 124:55796
 REFERENCE 2: 119:203068
 REFERENCE 3: 117:221961
 REFERENCE 4: 113:231504
 REFERENCE 5: 100:114289
 REFERENCE 6: 94:103288
 REFERENCE 7: 68:12087
 REFERENCE 8: 63:63003
 REFERENCE 9: 59:41423

=> d his

(FILE 'HOME' ENTERED AT 06:57:08 ON 19 SEP 2002)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 06:57:32 ON 19 SEP 2002

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 L1 30 S E3,E4,E6-E8
 E US2002-061617/AP,PRN
 E WO2002-US27953/AP,PRN
 E WO2002-US25609/AP,PRN
 E US2001-316151
 E US2001-316151/AP,PRN
 L2 0 S L1 AND HALOENAMINE
 L3 16 S HALOENAMINE
 L4 11 S L3 AND ALPHA
 L5 606 S AMINE#/CW (L) ENAMINE
 L6 240 S AMINE#/CW (L) HALO
 L7 4 S L5 AND L6
 L8 3 S L7 AND ALPHA
 L9 13 S L4,L8
 L10 5 S L3 NOT L9
 L11 103 S HALO(S)ENAMINE
 L12 154 S HALO(L)ENAMINE
 L13 48 S L11,L12 AND ALPHA
 L14 9 S L9 AND L13
 L15 13 S L9,L14
 L16 39 S L13 NOT L15
 L17 4 S L16 AND L6,L5
 L18 17 S L15,L17
 L19 35 S L16 NOT L18
 SEL DN AN 7 8 9 13 23 24
 L20 6 S L19 AND E1-E18
 L21 23 S L18,L20
 L22 24 S ALPHA() (CHLOROENAMINE OR BROMOENAMINE OR FLUOROENAMINE OR IOD
 L23 68 S ALPHA(S) (CHLORO OR BROMO OR FLUORO OR IODO) (S) ENAMINE
 L24 41 S ALPHA(S) HALO? (S) ENAMINE

L25 17 S L21 AND L22-L24
L26 23 S L21,L25
L27 105 S L22-L24 NOT L26
L28 97 S L27 NOT L19
L29 44 S L28 AND (NEW REAGENT OR REACTIVE INTERMEDIATE OR SYNTHESIS OR
SEL DN AN 9 23 26 27 30 34 38 39 41 44
L30 10 S E19-E48 AND L29
L31 33 S L26,L30
E ENAMINE/CT
E E4+ALL
L32 1739 S E8
L33 156 S L32 (L) (HALO? OR CHLORO? OR BROMO? OR FLUORO? OR IODO? OR CH
L34 131 S L33 NOT L13-L31
L35 4 S L34 AND (PARTIALLY FLUORINATED OR BROMINATION OR VERY MILD CO
SEL DN AN 2-3
L36 2 S L35 AND E1-E6
L37 37 S L31,L35
L38 76 S L32 (L) ALPHA
L39 56 S L38 NOT L33-L37
L40 37 S L37 AND L1-L39
L41 37 S L40 AND ?ENAMINE?
L42 37 S L41 AND (HALO? OR CHLOR? OR BROM? OR FLUOR? OR IODO? OR IODI?
L43 35 S L42 AND ALPHA
L44 2 S L42 NOT L43
L45 20436 S TRIETHYLAMINE OR TRIETHYL AMINE OR TRI ETHYLAMINE OR TRI ETHY
L46 20889 S TERTIARY AMINE
E TERTIARY AMINE/CT
E E6+ALL
L47 5470 S E2

FILE 'REGISTRY' ENTERED AT 07:46:31 ON 19 SEP 2002

L48 1 S 121-44-8

FILE 'HCAPLUS' ENTERED AT 07:47:18 ON 19 SEP 2002

L49 17005 S L48
L50 148 S DIETHYLAMINOETHANE OR DIETHYLAMINO ETHANE OR DIETHYL ETHANAMI
L51 47070 S L45-L47,L49,L50
L52 1 S PENTAVAL?(L) PHOSPHOROUS(S) (HALIDE OR CHLORIDE OR BROMIDE OR I
L53 106 S PHOSPHOROUS() (PENTABROMIDE OR PENTACHLORIDE OR PENTAFLUORIDE
L54 3643 S PHOSPHOR?() (PENTABROMIDE OR PENTACHLORIDE OR PENTAFLUORIDE OR
L55 6 S PHOSPHOR? PENTAIODIDE

FILE 'REGISTRY' ENTERED AT 07:55:17 ON 19 SEP 2002

L56 4 S 10026-13-8 OR 7789-69-7 OR 7647-19-0 OR 66656-29-9
L57 840 S P/ELS AND (CL OR BR OR I OR F)/ELS NOT (C OR N OR S OR SI OR
L58 526 S L57 NOT (CCS OR RIS OR PMS OR MNS)/CI
L59 48 S L58 AND NR>=2
L60 478 S L58 NOT L59
L61 279 S L60 AND 1/NC
L62 215 S L61 AND 1/P
L63 124 S L62 NOT (TIS OR AYS)/CI
L64 119 S L63 NOT 37CL
L65 114 S L64 NOT SE/ELS
L66 113 S L65 NOT CA/ELS
L67 108 S L66 NOT B/ELS
L68 107 S L67 NOT MN/ELS
L69 100 S L68 NOT ((CD OR GE)/ELS OR 35CL)
L70 98 S L69 NOT (TA OR NB)/ELS
L71 93 S L70 NOT 32P
L72 83 S L71 NOT (36CL OR 33P OR 18F OR 35P OR 74BR OR 35CL OR P35CL?
L73 81 S L72 NOT (P79BR? OR 79BR)
L74 72 S L73 NOT (CLP OR BRP OR IP OR FP OR P81BR?)
L75 13 S L74 AND 6/ATC

L76 13 S L56,L75
L77 59 S L74 NOT L76

FILE 'HCAPLUS' ENTERED AT 08:09:17 ON 19 SEP 2002

L78 2781 S L76
L79 5810 S L77
L80 9904 S L78,L79,L52-L55
SEL RN L22
DEL SEL

FILE 'REGISTRY' ENTERED AT 08:10:53 ON 19 SEP 2002

FILE 'HCAPLUS' ENTERED AT 08:10:53 ON 19 SEP 2002

SET SMARTSELECT ON
L81 SEL L22 1- RN : 509 TERMS
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 08:10:54 ON 19 SEP 2002

L82 509 S L81
L83 198 S L82 AND (N AND (CL OR BR OR I OR F))/ELS
L84 STR
L85 50 S L84
L86 25524 S L84 FUL
L87 STR L84
L88 2480 S L87 FUL SUB=L86
SAV L88 KUMAR061/A
L89 STR L87
L90 10183 S L89 FUL SUB=L86
SAV L90 KUMAR061A/A
L91 2124 S L88 AND 1/NC
L92 356 S L88 NOT L91

FILE 'HCAPLUS' ENTERED AT 08:17:39 ON 19 SEP 2002

L93 1163 S L88
L94 41 S L93 AND L51
L95 43 S L93 AND L80
L96 5714 S L90
L97 34 S L83 AND L96
L98 1 S L94 AND L95 AND L96
L99 72 S L88/P AND L94,L95,L97
L100 26 S L99 AND (L51(L) (RACT OR RCT OR RGT OR CAT)/RL OR L90(L) (RACT
L101 16 S L100 AND L51
L102 64 S L93 AND L3-L6,L11,L12,L22-L24,L32-L34
L103 3 S L102 AND L80
L104 15 S L43 AND L93-L103,L45-L47,L49-L55,L78-L80
L105 35 S L43,L104
L106 59697 S ACETONITRILE
L107 113831 S TETRAHYDROFURAN
L108 7836 S 1 4 DIOXANE
L109 12138 S METHYLENECHLORIDE OR METHYLENE CHLORIDE
L110 39945 S CHLOROFORM
L111 10466 S 1 2 DICHLOROETHANE
L112 64 S 1 2 DICHLORO ETHANE
L113 127691 S TOLUENE
L114 245181 S BENZENE

FILE 'REGISTRY' ENTERED AT 08:33:43 ON 19 SEP 2002

L115 8 S 75-05-8 OR 109-99-9 OR 123-91-1 OR 75-09-2 OR 67-66-3 OR 71-4

FILE 'HCAPLUS' ENTERED AT 08:33:54 ON 19 SEP 2002

L116 0 S L104 AND L106-L114,L115
L117 9 S L1 AND L2-L47,L49-L55,L78-L80,L93-L114
L118 220 S PHARMACIA?/PA,CS AND L2-L47,L49-L55,L78-L80,L93-L114

L119 1 S L118 AND L93
L120 0 S L118 AND L3-L6, L11, L12, L22-L24, L32-L34

FILE 'REGISTRY' ENTERED AT 08:37:50 ON 19 SEP 2002

L121 1 S L88 AND C6H12CLN/MF
L122 4 S L88 AND C12H16CLN/MF AND 46.150.18/RID
L123 1 S L122 NOT BUTEN
L124 59 S (C11H16N2O4 OR C11H15CLN2O3)/MF AND NC4/ES AND 1/NR
L125 42 S L124 AND ESTER
L126 30 S L124 AND 16.136.9/RID
L127 19 S L125 AND L126
L128 5 S L127 AND 1 METHYL
L129 25 S L126 NOT L128
L130 3 S L129 AND 1 METHYL
L131 1 S 77716-11-1
L132 3 S L124 AND CL/ELS
L133 20 S C10H13CLO2SI/MF AND 46.150.18/RID
L134 1 S L133 AND BENZOIC ACID AND 2 CHLORO 6
L135 7 S C10H12CL2OSI/MF AND 46.150.18/RID AND 1/NR
L136 1 S L135 AND BENZOYL CHLORIDE
L137 101 S C7H6O3/MF AND 46.150.18/RID AND 1/NR
L138 28 S L137 AND 2 HYDROXY
L139 27 S L138 AND BENZOIC
E BENZOIC ACID, 2-HYDROXY-/CN
L140 1 S E3
L141 67 S C7H5CLO2/MF AND 46.150.18/RID AND 1/NR
L142 7 S L141 AND 2 HYDROXY
L143 1 S 1441-87-8
L144 260 S C8H8O3/MF AND 46.150.18/RID AND 1/NR
L145 6 S L144 AND 2 HYDROXY AND METHYL ESTER
L146 1 S 119-36-8
L147 26 S L137 AND 4 HYDROXY AND BENZOIC
L148 1 S 99-96-7
L149 4 S L141 AND 4 HYDROXY
L150 1 S 28141-24-4
L151 9 S L144 AND 4 HYDROXY AND METHYL ESTER
L152 1 S 99-76-3
L153 378 S C8H9NO2/MF AND 46.150.18/RID AND 1/NR
L154 47 S L153 AND 4 HYDROXY
L155 1 S L154 AND BENZAMIDE AND N METHYL
L156 16 S C11H16CLNOSI/MF AND 46.150.18/RID AND 1/NR
L157 2 S L156 AND BENZAMIDE
L158 1 S 150108-45-5
L159 69 S C7H5NO4/MF AND 46.150.18/RID AND 1/NR
L160 12 S L159 AND 2 NITRO
L161 7 S L160 AND BENZOIC
L162 1 S 552-16-9
L163 12 S C7H4CLNO2/MF AND 46.150.18/RID AND 1/NR
L164 28 S C7H4CLNO3/MF AND 46.150.18/RID AND 1/NR
L165 1 S L164 AND BENZOYL CHLORIDE AND 2 NITRO
L166 169 S C8H7NO4/MF AND 46.150.18/RID AND 1/NR
L167 32 S L166 AND 2 NITRO
L168 7 S L167 AND BENZOIC ACID
L169 1 S 606-27-9
L170 198 S C8H8N2O3/MF AND 46.150.18/RID AND 1/NR
L171 32 S L170 AND 2 NITRO
L172 1 S L171 AND BENZAMIDE AND N METHYL

FILE 'HCAPLUS' ENTERED AT 09:26:12 ON 19 SEP 2002

L173 71 S L121
L174 0 S L131 AND L121

FILE 'REGISTRY' ENTERED AT 09:26:45 ON 19 SEP 2002

L175 45 S NCNC2/ES AND C10H15N3O4/MF AND 1/NR
L176 10 S L175 AND 1 METHYL
L177 1 S 128293-64-1
L178 0 S NCNC2/ES AND C10H14CLN3O3/MF AND 1/NR

FILE 'HCAPLUS' ENTERED AT 09:30:03 ON 19 SEP 2002

L179 0 S L177 AND L173
L180 1 S L123
L181 0 S (L134,L136,L158,L140,L143,L146,L148,L150,L152,L155,L162,L165,
L182 1 S L134 AND L136,L158
L183 1 S L136 AND L158
L184 1 S L182,L183
L185 529 S L140 AND L143,L146
L186 13 S L143 AND L146
L187 8 S L185 AND L186
L188 0 S L146/P AND L187
L189 554 S L148 AND (L150,L152,L155)
L190 3 S L150 AND L152,L155
L191 2 S L189 AND L190
L192 0 S (L152/P OR L155/P) AND L191
L193 59 S L162 AND L165,L169,L172
L194 2 S L165 AND L169,L172
L195 0 S L193 AND L194
L196 0 S L1 AND L173,L123
L197 2 S L1 AND L131,L177,L134,L136,L158,L140,L143,L146,L148,L150,L152
L198 2 S L184,L197
L199 37 S L105,L198
L200 0 S N 1 CHLORO 2 METHYLPROP 1 ENYL N METHYL AMINOMETHYL?
L201 10 S CHLORO(L)METHYLPROP?(L)?AMINOMETHYL?
L202 0 S L180 AND ?STYREN?

FILE 'HCAPLUS' ENTERED AT 09:42:46 ON 19 SEP 2002

FILE 'REGISTRY' ENTERED AT 09:43:40 ON 19 SEP 2002

L203 10 S 1 CHLORO AND 2 METHYLPROPEN? AND N/ELS
L204 780 S L86 AND 1 CHLORO AND N
L205 260 S L88 AND L204
L206 1 S L205 AND AMINOMETHYL
L207 22 S L205 AND AMINO METHYL
L208 129 S L205 AND 46.150.18/RID NOT L207
L209 65 S L208 AND 1/NR
L210 47 S L209 AND 1/CL
L211 109 S L205 NOT L206-L210
L212 12 S L211 AND NR>=1
L213 97 S L211 NOT L212
L214 59 S L213 NOT (S OR P OR SI OR O)/ELS
L215 45 S L214 AND 1/CL
L216 17 S L214 AND PROPEN?